Phase Diagram Of Hydrogen

Methods for Phase Diagram Determination
The Phase Diagram of Hydrogen in Ultra Thin Films
Hydrides for Energy Storage
Correlations in Condensed Matter under Extreme Conditions
Proceedings of the Thirteenth International Conference on Chemical Vapor Deposition
Phase Diagrams of Binary Hydrogen Alloys
The Zirconium-hydrogen System at High Hydrogen Contents
Thermodynamic Diagrams for High Temperature Plasmas of Air, Air-Carbon, Carbon-Hydrogen Mixtures, and Argon
Experiments on a Strongly Correlated Material
Diagramme Zur Chemie und Thermodynamik Von Hochtemperaturplasmen Für Luft, Luft Mit Kohlenstoff, Kohlenstoff-Wasserstoff-Gemische und Argon
THERMODYNAMIC Diagrams for High Temperature Plasmas of Air, Air-carbon, Carbon-hydrogen Mixtures, and Argon
Applications of Phase Diagrams in Metallurgy and Ceramics
LOW-TEMPERATURE VAPOR-LIQUID EQUILIBRIA IN TERNARY AND QUATERNARY SYSTEMS CONTAINING HYDROGEN, NITROGEN, METHANE

AND ETHANE.
Los Alamos Science
Chemistry in Space
Low-temperature vapor-liquid equilibria in ternary and quaternary systems containing hydrogen, nitrogen, methane and ethane
Selected Properties of Hydrogen (engineering Design Data)
Handbook of Hydrogen Storage
Interrelations Between Phase Diagrams and Hydriding Properties for Alloys Based on the Intermetallic Compound FeTi
Hydrogen Redistribution in Zircaloy-2 Under Thermal and Mechanical Stress Gradients
Liquid-liquid Phase Transition in Hydrogen by Coupled Electron-ion Monte Carlo Simulations
Quantum Monte Carlo Study of the High Pressure Phases of Solid Hydrogen
The Metal-Hydrogen System
Hydrogen in Metals II
Discovery of Novel Complex Metal Hydrides for Hydrogen Storage Through Molecular Modeling and Combinatorial Methods
Phase Diagrams of the Elements
A Study of the Low Temperature Phase Diagram of Low Concentrations of Hydrogen in Niobium
The Index to Binary Phase Collections
Hydrogen Materials Science and Chemistry of Metal Hydrides
The Phase Diagram of the System Ammonia-hydrogen Sulfide
High Pressure Science And Technology -

DIAZ BOND

Methods for Phase Diagram Determination Springer Hydrogen is the smallest impurity atom that can be implanted in a metallic host. Its small mass and strong interaction with the host electrons and nuclei are responsible for many anomalous and interesting solid state effects. In addition, hydrogen in metals gives rise to a number of technological problems such as hydrogen embrittlement , hydrogen storage, radiation hardening, first wall problems associated with nuclear fusion reactors, and degradation of the fuel cladding in fission reactors. Both the fundamental

effects and applied problems have stimulated a great deal of inter est in the study of metal hydrogen systems in recent years. This is evident from a growing list of publications as well as several international conferences held in this field during the past decade. It is clear that a fundamental understanding of these problems re quires a firm knowledge of the basic interactions between hydrogen, host metal atoms, intrinsic lattice defects and electrons. This understanding is made particularly difficult by hyrogen's small mass and by the large lattice distortions that accompany the hydrogenation process. The purpose of the "International Symposium on the Electronic Structure and Properties of Hydrogen in Metals" held in Richmond, Virginia, March 4-6, 1982 was to increase our fundamental under standing of hydrogen in metals. Such knowledge is essential in solving technologicall y important questions. The symposium con sisted of twenty-two invited papers and seventy-two contributed poster presentations and attracted nearly 150 participants from thirteen countries. The proceedings of this symposium constitute this book.

The Phase Diagram of Hydrogen in Ultra Thin Films Phase Diagrams of Binary Hydrogen AlloysThe Phase Diagram of Hydrogen in Ultra Thin FilmsSelected Properties of Hydrogen (engineering Design Data)Thermodynamic Diagrams for High Temperature Plasmas of Air, Air-Carbon, Carbon-Hydrogen Mixtures, and Argon Metal hydrides are of inestimable importance for the future of hydrogen energy. This unique monograph presents a clear and comprehensive description of the bulk properties of the metal-hydrogen system. The statistical thermodynamics is treated over a very wide range of pressure, temperature and composition. Another prominent feature of the book is its elucidation of the quantum mechanical behavior of interstitial hydrogen atoms, including their states and motion. The important topic of hydrogen interaction with lattice defects and its materials-science implications are also discussed thoroughly. This second edition has been substantially revised and updated. Hydrides for Energy Storage The Electrochemical Society In order to elucidate the phase

diagram of the Zr--H system at high hydrogen contents, a pressure-compositionte mperature study of this system in the temperature range 550 to 850 deg C was carried out from ZrH to ZrH2. From the obtained isotherms, the position of the boundary between the two-phase (beta + delta) region and the single phase delta region was more precisely defined (where beta designates the hydrogen stabilized high temperature zirconium phase, and delta the cubic hydride phase). The isotherm also show no evidence of a two-phase hydride region (cubic + tetragonal hydrides coexisting) in this temperature range, as has been observed at room temperature. (auth).

Correlations in Condensed Matter under Extreme Conditions

John Wiley & Sons

Phase diagrams are "maps" materials scientists often use to design new materials. They define what compounds and solutions are formed and their respective compositions and amounts when several elements are mixed together under a certain temperature and pressure. This monograph is the most comprehensiv e reference book on experimental methods for

phase diagram determination. It covers a wide range of methods that have been used to determine phase diagrams of metals, ceramics, slags, and hydrides. * Extensive discussion on methodologies of experimental measurements and data assessments * Written by experts around the world, covering both traditional and combinatorial methodologies * A must-read for experimental measurements of phase diagrams

Proceedings of the Thirteenth International Conference on Chemical Vapor Deposition

Elsevier

The phase diagram of high-pressure hydrogen is of great interest for fundamental research, planetary physics, and energy applications. A first-order phase transition in the fluid phase between a molecular insulating fluid and a monoatomic metallic fluid has been predicted. The existence and precise location of the transition line is relevant for planetary models. Recent experiments reported contrasting results about the location of the transition. Theoretical results based on density functional theory are also very scattered. We report highly accurate coupled electron-ion

Monte Carlo calculations of this transition, finding results that lie between the two experimental predictions, close to that measured in diamond anvil cell experiments but at 25-30 GPa higher pressure. Here, the transition along an isotherm is signaled by a discontinuity in the specific volume, a sudden dissociation of the molecules, a jump in electrical conductivity, and loss of electron localization.

Phase Diagrams of Binary Hydrogen Alloys

Elsevier

Hydriding alloys based on the intermetallic compound FeTi have potential for the safe and convenient storage of hydrogen, both for mobile and stationary applications. In spite of its simple formula, the hydriding behavior of FeTi is quite complex and a strong function of alloy microstructure. The alloy microstructure, in turn, depends on composition, not only deviations from stoichiometry but also various impurities. In this paper we discuss some of the interrelations among composition, microstructure, and hydriding behavior that can be related to phase diagram information. In particular, we discuss the Fe--Ti, Fe--Ti--O, and Fe--Ti--

Mn phase diagrams and their relationships to hydriding properties. The use of hydriding data to infer metal-hydrogen phase diagrams is also briefly discussed.

The Zirconium-hydrogen System at High Hydrogen Contents

Springer

In September, 1999, with the generous support of NATO, scientists from 18 different nations gathered in Katsiveli, Yalta, Ukraine at the NATO Advanced Research Workshop on Hydrogen Materials Science and Chemistry of Metal Hydrides to present their research and to discuss world energy problems and possible solutions, interactions of hydrogen with materials, the role of hydrogen in materials science, and the chemistry of metal hydrides. High level and highly professional presentations were accompanied by a great deal of discussion and debate of the issues from both fundamental and global perspectives. The result was a large number of new collaborations, new directions, and better understanding of energy and materials issues. The research presented at this meeting can be found in this volume. These papers range from global perspectives

such as the new vision of energy and how hydrogen fits into that future, to reviews such as a look at nickel hydride over the last 40 years, to very specific current research. A large number of papers are included on hydrogen and materials. These papers include articles on properties such as superconductivity, diffusion EMF, magnetic properties, physico chemical properties, phase composition, and permeability as a result of the interaction with or incorporation of hydrogen. Also included are papers discussing the use of hydrogen as a processing or alloying agent. The use of hydrogen in the synthesis of battery electrode materials, composite materials, and alloys is also presented. *Thermodynamic Diagrams for High Temperature Plasmas of Air, Air-Carbon, Carbon-Hydrogen Mixtures, and Argon* World Scientific Phase Diagrams of Binary Hydrogen AlloysThe Phase Diagram of Hydrogen in Ultra Thin FilmsSelected Properties of Hydrogen (engineering Design Data)Thermodynamic Diagrams for High Temperature Plasmas of Air, Air-Carbon, Carbon-Hydrogen Mixtures, and ArgonElsevier *Experiments on a Strongly Correlated*

Material Elsevier Hydrides for Energy Storage documents the proceedings of an International Symposium held in Geilo, Norway on August 14-19, 1977. This book discusses the thermodynamics of metal, alloy and intermetallic/hydrogen systems; localization and diffusion of hydrogen in lanthanum-nickel compounds; kinetics of hydrogen absorption and desorption; and nuclear magnetic resonance studies of metal hydrides. The calculated heats of formation of metal and metal alloy hydrides; hydrogen absorption into rare earth intermetallic compounds; plateau pressure of RE Ni5 and RE Co5 hydrides; and hydride formation of C14-type Ti alloy are also elaborated. This text likewise covers the mixing effects of two different types of hydrides; hydrogen storage electrode systems; and applications of metal hydrides. This publication is intended for chemists concerned with the fundamental properties of hydrides.

Diagramme Zur Chemie und Thermodynamik Von Hochtemperaturplasmen Für Luft, Luft Mit Kohlenstoff, Kohlenstoff-Wasserstoff-Gemische und Argon

Springer Science & Business Media Thermodynamic Diagrams for High Temperature Plasmas of Air, Air-Carbon, Carbon-Hydrogen Mixtures, and Argon provides information relating to the properties of equilibrium gas plasmas formed from hydrocarbons, from air without argon, from pure argon, and from mixtures of air and carbon at various compositions, temperatures and pressures. The data are presented in graphical rather than tabular form to provide a clearer picture of the plasma processes investigated. This book is composed of four chapters, and begins with the introduction to the characteristics of plasmas, with emphasis on their thermodynamic properties. The succeeding chapter deals with the theoretical basis of the computations of thermodynamic properties using a system of equations derived from quantized Boltzmann statistics. These topics are followed by discussions on the calculation of equilibrium compositions and the thermodynamic values for thermal plasmas. The final chapter describes proposed models on which the calculations are based. This book will prove useful to chemical technologists

and researchers.

THERMODYNAMIC Diagrams for High Temperature Plasmas of Air, Air-carbon, Carbon-hydrogen Mixtures, and Argon

Springer

The behavior of solid and liquid matter at high pressures and temperatures is best described in a phase diagram, which shows the regions of stability of different phases of the material. Thanks to the diamond-anvil cell, which has made possible much higher pressures, and to new and very accurate theoretical models and methods, Phase Diagrams of the Elements presents the most up-to-date information on the phase behavior of all the chemical elements from hydrogen to fermium. The book summarizes, with the aid of tables and illustrations, the experimental data and the theoretical calculations. Each element is discussed in a separate section. Other chapters deal with methods, the liquid-vapor transition, and an overview of the elements. While comprehensively reviewing all that has been done in this important area, the author also points to questions that need much more experimental and theoretical work.

Applications of Phase Diagrams in Metallurgy

and Ceramics Springer The metal-insulator transition(MIT) in vanadium dioxide(VO2) has attracted waves of attention after its rst observation by Morin in 1959. There are several reasons for the interest in this material. First, its metal-insulator transition is at an easily accessible temperature which allows investigators to study the eect of strong elec- tronic correlations with little eort. Second reason is VO2 oers many applications, although most of them are mundane, a few may have signicant eects on dierent areas of technology. However, even after over half a century there is still a debate about the nature of the MIT and non of the applications proposed have been realized. The main culprit for this is the diculties in studying the bulk crystals of VO2. In bulk crystals, defects in the crystal, impurities and domain structure causes irrepro-ducible results. This combined with the theoretical challenges made studying VO2 and realization of applications impractical. However, recent discovery of the growth technique for growing the nano-scale crystals, revitalized the interest in VO2. In this dissertation I present the experimental studies that

we performed on VO2. I discussed the ndings from three major studies we performed; photorespons e, nd- ing the strain-temperature phase diagram and hydrogen doping of VO2. We used scanning photocurrent microscopy technique to reveal the light-matter interaction in VO2. Suspended nanobeam devices are used in the experiments and results revealed that photorespons e of VO2 is dominated by the thermal eects and there is no pho- tovoltaic contribution. Results are published in Nature Nanotechnolo gy in 2012 . In the second study, we determined the strain-temperature phase stability diagram of VO2. This is the rst ever determination of the phase diagram of a solid state phase transition. Also our studies revealed that the triple point coincides with the critical point, which has important implications for both theoretical studies of the MIT in VO2 and for its applications. Results of this study is published in Nature in 2013. Last study presented here is the hydrogen doping of VO2. There is not much known about hydrogenation of VO2. However our initial studies revealed very high anisotropy of diusion and mechanism

other than diusion eecting the hydrogen motion in the VO2 crystal. There is also a chapter on previous studies and a general introduction to the MIT in VO2. Appendices contain detailed information about the experiment setups, crystal growth techniques and device fabrication techniques. I believe studies presented here with the recent advances in the eld had an important contribution to our understanding of the MIT in VO2 and brought us closer to the realization of tantalizing applications. *LOW-TEMPERATURE VAPOR-LIQUID EQUILIBRIA IN TERNARY AND QUATERNARY SYSTEMS CONTAINING HYDROGEN, NITROGEN, METHANE AND ETHANE.* Springer Science & Business Media This important book provides an introduction to the liquid state. A qualitative description of liquid properties is first given, followed by detailed chapters on thermodynamics, liquid structure in relation to interaction forces and transport properties such as diffusion and viscosity. Treatment of complex fluids such as anisotropic liquid crystals and polymers, and of technically important topics such as non-

Newtonian and turbulent flows, is included. Surface properties and characteristics of the liquid-vapour critical point are also discussed. While the book focuses on classical liquids, the final chapter deals with quantal fluids. Los Alamos Science World Scientific The dynamic field of extraterrestrial chemistry brings together ideas of chemistr, astrophysics, and biology to the study of molecules between stars, around stars, and on plantes. This book serves as an introduction to chemial processes under ¿unearthly¿ and hence usually extreme conditions (temperature, pressure, high or low density, bombardment by cosmic rays), and their impact on the early development of our solar system, as well as providing a deeper understanding of processes in earthly regions where conditions approach those of extraterrestrial areas. A unique and extraordinary perspective written with chemists in mind. An excellent practical book for inorganic, and physical chemists, spectroscopists, astronomers, and libraries. From the contents: * Introduction and technical notes * Origin and development of the universe * Stars * The interstellar

medium * The solar system * Exoplanets * The origin of life Chemistry in Space Elsevier Owing to the limited resources of fossil fuels, hydrogen is proposed as an alternative and environment-friendly energy carrier. However, its potential is limited by storage problems, especially for mobile applications. Current technologies, as compressed gas or liquefied hydrogen, comprise severe disadvantages and the storage of hydrogen in lightweight solids could be the solution to this problem. Since the optimal storage mechanism and optimal material have yet to be identified, this first handbook on the topic provides an excellent overview of the most probable candidates, highlighting both their advantages as well as drawbacks. From the contents: ¿ Physisorption ¿ Clathrates ¿ Metal hydrides ¿ Complex hydrides ¿ Amides, imides, and mixtures ¿ Tailoring Reaction Enthalpies ¿ Borazan ¿ Aluminum hydride ¿ Nanoparticles A one-stop reference on all questions concerning hydrogen storage for physical and solid state chemists, materials scientists, chemical engineers, and physicists. Low-

temperature vapor-liquid equilibria in ternary and quaternary systems containing hydrogen, nitrogen, methane and ethane
Springer Science & Business Media
This book addresses a wide range of topics relating to the properties and behavior of condensed matter under extreme conditions such as intense magnetic and electric fields, high pressures, heat and cold, and mechanical stresses. It is divided into four sections devoted to condensed matter theory, molecular chemistry, theoretical physics, and the philosophy and history of science. The main themes include electronic correlations in material systems under extreme pressure and temperature conditions, surface physics, the transport properties of low-dimensional electronic systems, applications of the density functional theory in molecular systems, and graphene. The book is the outcome of a workshop held at the University of Catania, Italy, in honor of Professor Renato Pucci on the occasion of his 70th birthday. It includes selected invited contributions from collaborators and co-authors of Professor Pucci during his long and

successful career, as well as from other distinguished guest authors.

Selected Properties of Hydrogen (engineering Design Data)

Univ of California Press

UOP LLC, a Honeywell Company, Ford Motor Company, and Striatus, Inc., collaborated with Professor Craig Jensen of the University of Hawaii and Professor Vidvuds Ozolins of University of California, Los Angeles on a multi-year cost-shared program to discover novel complex metal hydrides for hydrogen storage. This innovative program combined sophisticated molecular modeling with high throughput combinatorial experiments to maximize the probability of identifying commercially relevant, economical hydrogen storage materials with broad application. A set of tools was developed to pursue the medium throughput (MT) and high throughput (HT) combinatorial exploratory investigation of novel complex metal hydrides for hydrogen storage. The assay programs consisted of monitoring hydrogen evolution as a function of temperature. This project also incorporated theoretical methods to help select candidate materials families for testing. The Virtual High

Throughput Screening served as a virtual laboratory, calculating structures and their properties. First Principles calculations were applied to various systems to examine hydrogen storage reaction pathways and the associated thermodynamics. The experimental program began with the validation of the MT assay tool with NaAlH4/0.02 mole Ti, the state of the art hydrogen storage system given by decomposition of sodium alanate to sodium hydride, aluminum metal, and hydrogen. Once certified, a combinatorial 21-point study of the NaAlH4 - LiAlH4 - Mg(AlH4)2 phase diagram was investigated with the MT assay. Stability proved to be a problem as many of the materials decomposed during synthesis, altering the expected assay results. This resulted in repeating the entire experiment with a mild milling approach, which only temporarily increased capacity. NaAlH4 was the best performer in both studies and no new mixed alanates were observed, a result consistent with the VHTS. Powder XRD suggested that the reverse reaction, the regeneration of the alanate

from alkali hydride, Al and hydrogen, was hampering reversibility. The reverse reaction was then studied for the same phase diagram, starting with LiH, NaH, and MgH2, and Al. The study was extended to phase diagrams including KH and CaH2 as well. The observed hydrogen storage capacity in the Al hexahydrides was less than 4 wt. %, well short of DOE targets. The HT assay came on line and after certification with studies on NaAlH4, was first applied to the LiNH2 - LiBH4 - MgH2 phase diagram. The 60-point study elucidated trends within the system locating an optimum material of 0.6 LiNH2 - 0.3 MgH2 - 0.1 LiBH4 that stored about 4 wt. % H2 reversibly and operated below 220 °C. Also present was the phase Li4(NH2)3BH4, which had been discovered in the LiNH2 - LiBH4 system. This new ternary formulation performed much better than the well-known 2 LiNH2 - MgH2 system by 50 °C in the HT assay. The Li4(NH2)3BH4 is a low melting ionic liquid under our test conditions and facilitates the phase transformations required in the hydrogen storage reaction, which no longer relies on a higher energy solid state reaction pathway.

Further study showed that the 0.6 LiNH2 - 0.3 MgH2 - 0.1 LiBH4 formulation was very stable with respect to ammonia and diborane desorption, the observed desorption was from hydrogen. This result could not have been anticipated and was made possible by the efficiency of HT combinatorial methods. Investigation of the analogous LiNH2 - LiBH4 - CaH2 phase diagram revealed new reversible hydrogen storage materials 0.625 LiBH4 + 0.375 CaH2 and 0.375 LiNH2 + 0.25 LiBH4 + 0.375 CaH2 operating at 1 wt. % reversible hydrogen below 175 °C. Powder x-ray diffraction revealed a new structure for the spent materials which had not been previously observed. While the storage capacity was not impressive, an important aspect is that it boron appears to participate in a low temperature reversible reaction. The last major area of study also focused on activating boron-based materials in order to exploit the tremendous gravimetric capacity of LiBH4. A number of LiNH2 - LiBH4 - transition metal (TM) systems were investigated for the following reasons. No additional leads were discovered in this system.

Another major project activity was the assembly of a high throughput synthesis system. The automated synthesizer was set up in a glovebox and was capable of handling liquids and powders and carrying out sealed block syntheses up to 250 °C. Unfortunately, the synthesizer could not handle the delivery of the fine powders required fro hydrogen storage applications. Although the powder delivery system was overhauled and redesigned several times, this problem was never remedied. *Handbook of Hydrogen Storage* John Wiley & Sons Vol. 2. Interrelations Between Phase Diagrams and Hydriding Properties for Alloys Based on the Intermetallic Compound FeTi Springer Variational and Diffusion Monte Carlo are powerful computational methods which can afford accurate estimates of the ground state properties of quantum many-body problems. We have applied these Monte Carlo methods to the high pressure phases of solid hydrogen to elucidate those parts of the phase diagram where experimental results are inconclusive or lacking. The method allows us to treat both electrons and protons as quantum

particles by incorporating them in the trial wavefunction and avoids the Born-Oppenheimer and harmonic approximation s. Our trial wavefunction uses single-body solutions from a mean-field calculation coupled with standard pair potential terms to achieve the most accurate results to date. Equally accurate results were realized for calculations in the disparate insulating molecular and metallic atomic regime. We performed a study of the possible ground state structures of the atomic metallic phase of hydrogen which identifies a new family of low energy atomic structures. Another study was done on the molecular phase over the range of pressures (40-180GPa) where recent experiments have observed spectral discontinuities and other interesting new phenomena. Particular attention was directed to determining the equation of state and orientational ordering. We find that molecular hydrogen adopts a lower symmetry insulating structure over a wide range of pressure. The results of the atomic and molecular studies are combined to draw conclusions about the molecular-atomic transition and other details about the high pressure

phase diagram. *Hydrogen Redistribution in Zircaloy-2 Under Thermal and Mechanical Stress Gradients* Metal Hydrides focuses on the theories of hydride formation as well as on experimental procedures involved in the formation of hydrides, the reactions that occur between hydrides and other media, and the physical and mechanical properties of the several classes of hydrides. The use of metal hydrides in the control of neutron energies is discussed, as are many other immediate or potential uses, e.g., in the production of high-purity hydrogen and in powder metallurgy. It is hoped that this book will serve as a valuable reference to students, research professors, and industrial researchers in metal hydrides and in allied fields. Selected chapters may serve specialists in other fields as an introduction to metal hydrides. The information contained herein will also be of lasting and practical value to the metallurgist, inorganic chemist, solid-state physicist, nuclear engineer, and others working with chemical or physical processes involving metal-hydrogen systems.

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