The Abdus Salam
International Centre for Theoretical Physics

United Nations
Educational, Scientific and
Cultural Organization

IAEA
International Atomic Energy Agency

Joint ICTP-IAEA Advanced School on the Role of Nuclear Technology in Hydrogen-Based Energy Systems

13 - 18 June 2011
(Trieste, Italy)

PROGRAMME

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POSTER ABSTRACTS

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The Abdus Salam
International Centre for Theoretical Physics

Joint ICTP-IAEA Advanced School on the Role of Nuclear Technology in Hydrogen-Based Energy Systems

Organizer(s): IAEA: A. Zeman, I. Khamis, M. Haji-Saeid. ICTP: R. Gebauer
Trieste - Italy, 13 - 18 June 2011

Venue: Adriatico Guest House Giambiagi Lecture Hall

Preliminary Programme

Monday, 13 June 2011 (Chair M. Steen) (Room:Adriatico Guest House Giambiagi Lecture Hall)

13 June 2011

08:00 - 09:00 **Registration**

09:00 - 09:15 **Opening - I. Khamis**

09:15 - 09:30 **ICTP introduction - R. Gebauer**

09:30 - 10:30 **M. Steen** / *(EC, Joint Research Centre, Le Petten)*
Status of hydrogen economy world wide prospective

10:30 - 11:00 --- Coffee Break ---

11:00 - 12:00 **I. Khamis** / *(IAEA, Vienna)*
IAEA initiatives on hydrogen related activities

12:00 - 13:30 --- Lunch ---

13:30 - 14:30 **M. Steen** / *(IAEA, Vienna)*
European program related to the hydrogen economy

14:30 - 15:30 **J. Huot** / *(Universite du Quebec a Trois-Rivieres, Canada)*
Hydrogen storage research programs in Canada and North America

15:30 - 16:00 --- Coffee Break ---

16:00 - 17:00 **K. Verfondern** / *(Research Centre Julich, Germany)*
Hydrogen Economy and the Role of Nuclear Power

17:00 - 18:00 **Posters session (display of individual posters)**

19:00 - 21:00 **Welcome Reception**

Tuesday, 14 June 2011 (Chair I. Khamis) (Room:Adriatico Guest House Giambiagi Lecture Hall)

14 June 2011

08:30 - 09:30 **K. Verfondern** / *(Research Centre Julich, Germany)*
Hydrogen Production Systems

09:30 - 10:30 **Nuclear Process Heat Reactors** / *(Research Centre Julich, Germany)*
K. Verfondern

10:30 - 11:00 --- Coffee Break ---

11:00 - 12:00 **U. Malshe** / *(Bhabha Atomic Research Centre, Mumbai)*
HEEP: The Tool for Comprehensive Cost Assessment of Hydrogen from Nuclear Energy: A brief Introduction

12:00 - 13:30 --- Lunch ---

13:30 - 15:30 **U. Malshe** / *(Bhabha Atomic Research Centre, Mumbai)*
HEEP software demonstrations - part 1

15:30 - 16:00 --- Coffee Break ---

16:00 - 17:00 **U. Malshe** / *(Bhabha Atomic Research Centre, Mumbai)*
HEEP software demonstrations - part 2

17:00 - 18:00 **Poster Sessions**

Wednesday, 15 June 2011 (Chair: D. Fruchart) (Room:Adriatico Guest House Giambiagi Lecture Hall)

15 June 2011

08:30 - 09:30 **J. Huot** / *(Universite du Quebec a Trois-Rivires, Canada)*
Basic crystallography for neutron and X-ray diffraction

09:30 - 10:30 **P. Moretto**
Overview of the technology state-of-advancement and challenges for the hydrogen storage (both stationary and for transport applications)

10:30 - 11:00 --- Coffee Break ---

11:00 - 12:00 **J. Huot** / *(Universite du Quebec a Trois-Rivieres, Canada)*
Basics of metal hydrides

12:00 - 13:30 --- Lunch ---

14:00 - 17:00 **Technical Tour - ELETTRA synchroton facility**

Thursday, 16 June 2011 (Chiar: J. Huot) (Room:Adriatico Guest House Giambiagi Lecture Hall)

16 June 2011

08:30 - 09:30 **D. Fruchart** / *(Institute Neel, Grenoble)*
Hydrogen in metals, various scale impacts on the structural, mechanical & magnetic properties of alloys

09:30 - 10:30 **D. Fruchart** / *(Institute Neel, Grenoble)*
Fundamental bases of neutron scattering and Comparative review of atomic and magnetic ordering in intermetallic compounds using various scale probes - part 1

10:30 - 11:00 --- Coffee Break ---

11:00 - 12:00 **D. Fruchart** / *(Institut Neel, Grenoble)*
Comparative review of atomic and magnetic ordering in intermetallic compounds using various scale probes - part 2: neutron scattering, Mössbauer, μ+SR, PAC, XANES-EXAFS-XMCD and NMR spectroscopies

12:00 - 13:30 --- Lunch ---

13:30 - 14:30 **J. Huot** / *(Universite du Quebec, Canada)*
Use of neutron diffraction for development of metal hydrides

14:30 - 15:30 **M. Kurdiachova** / *(St. Petersburg University, Russia)*
Ab-initio calculations of hydrogen storage systems - part 1

15:30 - 16:00 --- Coffee Break ---

16:00 - 18:00 **Poster Session (Evaluation)**

Friday, 17 June (Chair: R. Coppola) (Room:Adriatico Guest House Giambiagi Lecture Hall)

17 June 2011

08:30 - 09:30 **M. Kurdiachova** / *St. Petersburg University, Russia)*
Ab-initio calculations of hydrogen storage systems - part 2

09:30 - 10:30 **S. Fabris** / *(SISSA, Trieste)*
Computational modelling of catalytic materials for hydrogen-based technologies

10:30 - 11:00 --- Coffee Break ---

11:00 - 12:00 **G. Scherer** / *(Paul Scherrer Institute, PSI, Villigen)*
General introduction to fuel cells

12:00 - 13:30 --- Lunch ---

13:30 - 14:30 **G. Scherer** / *(Paul Scherrer Institute, PSI, Villigen)*
Proton-conducting membranes as solid electrolytes by radiation grafting

15:30 - 16:00 --- Coffee Break ---

16:00 - 17:00 **R. Coppola** / *(ENEA, Rome)*
Neutron diffraction studies of electrodes for innovative fuel cells of industrial interest

Saturday, 18 June 2011 (Chair: G. Scherer) (Room:Adriatico Guest House Giambiagi Lecture Hall) (**Saturday**)

18 June 2011

08:30 - 09:30 **M. Kazemian Abyaneh** / *(Islamic Azad University, Garmsar)*
Scanning photoemission microscope: A powerful tool for studies on Fuel cells and catalysis supporting material

09:30 - 10:30 **D. Fruchart** / *(Institut Neel, Grenoble)*
Reversible hydrogen storage in MgH2: from myth to realty

10:30 - 11:00 --- Coffee Break ---

11:00 - 12:00 **A. Gianoncelli** / *(ELETTRA, Sincrotrone, Trieste)*
In situ Electrochemical Studies of Fuel Cells by Soft-X-Ray Spectromicroscopy

12:00 - 12:30 **Poster Presentations**

12:30 - 13:00 **Participants Certificate Awards**

13:00 - 14:00 --- Lunch and Departure ---

Joint ICTP-IAEA Advanced School on the Role of Nuclear technology in Hydrogen-Based Energy Systems

13 - 18 June 2011

ABSTRACT TITLES

1. **Brigita Abakeviciene**
   Microstructure of NiO-YSZ cermets prepared by screen-printing - Impact of hydrogen reduction temperature

2. **Atindra Mohan Banerjee**
   Kinetics of sulfuric acid decomposition over iron oxide based catalysts

3. **I.F. Bouguenna**
   The Management of Water in a Fuel Cell with Membrane Exchanger of Protons (PEMFC)

4. **Monique Osório Talarico da Conceição**
   Hydrogen sorption kinetics of MgH_2 doped with Pd and V particles performed by mechanical milling

5. **K.T. Eyyubov**
   Radiolytic processes of hydrogen formation from n-C_6H_{14}+H_2O mixture

6. **J. Gajević**
   Electronic screening metals

7. **Daniel González Rodríguez**
   Conceptual design model of the sulfur-iodine S-I therochemical water splitting process for hydrogen production using nuclear heat source

8. **S.M. He**
   In-situ determination of aging precipitation in deformed Fe-Cu and Fe-Cu-B-N alloys by time resolved small-angle neutron scattering

9. **Cynthia Ibeto**
   Feasibility of large scale production and utilization of hydrogen fuel in Sub-Saharan Africa

10. **Pragya Jain**
    Investigating the improvements in hydrogenation properties of Mg films by Ti/ Zr layer addition using NRA and ERDA

11. **Zulkarnain Jalil**
    Hydrogen storage properties of MgH_2 alloys produced by high energy ball milling

12. **Galina Lazareva**
Kinetics of gas desorption from highly defected material photovoltaic plant at Trieste (Italy) using artificial Performance prediction of 20 kWp grid-connected neural network

13. **M. Lelis**
Substrate Effects on formation and hydrogenation of MG-NI films

14. **A. Mellit**
Ann-based prediction of a 20 kWp grid-connected photovoltaic power at Trieste (Italy)

15. **M. Eswaramoorthy**
Study on solar thermoelectric hydrogen energy system

16. **Jonatan Pérez-Alvarez**
$CoTiO_3$-TiO_2 thin films prepared by crossed beam pulsed laser deposition for hydrogen production by electrolysis

17. **Rafaella Martins Ribeiro**
Hydride formation and effects of hydrogen on the mechanical properties of Zirconum rich alloys

18. **B.A. Talagañis**
Novel device for simultaneous volumetric and X-rays diffraction measurements

19. **Mohd Syukri Yahya**
Overview of hydrogen economy R&D activities in Malaysia

20. **Barbara Susete Yaeggy Alvarez**
A Quantization of Bosonic String

Microstructure of NiO-YSZ Cermets Prepared by Screen-printing – Impact of Hydrogen Reduction Temperature

Brigita Abakeviciene[1], Sigitas Tamulevicius[1], Edvinas Navickas[1], Igoris Prosycevas[1]
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Cermets of yttria stabilized zirconia with nickel (YSZ-Ni) are one of the most promising materials for the anode-supported solid oxide fuel cells (SOFC). The screen-printing technology was used to produce NiO-YSZ cermets by mixing commercial NiO (7 μm particle size) and YSZ (3 μm particle size) powders in variable composition ratio respectively from 35 % : 65 % to 70 % : 30 % with 5 % increments. NiO-YSZ powders were mixed with suitable organic additives and printed on Al_2O_3 substrate. A 18 μm thick cermets were then calcined at 1350 °C for 2 h. Hydrogen reduction on NiO-YSZ anodes was investigated at 300 °C, 600 °C, 800 °C and 1000 °C reduction temperatures for 1 h and at 800 °C for 3 h. The microstructure, elemental composition of unreduced and reduced NiO-YSZ cermets with different porosity was analyzed using scanning electron microscope (SEM) and X-ray energy dispersive method (EDX). X-ray diffraction (XRD) method was employed to identify and quantify the phases of anodic cermets before and after the reduction performed at different temperatures. It was found that NiO-YSZ cermets consist mainly of cubic yttria stabilized zirconia and nickel oxide phases and additional cubic nickel phase resulting from NiO to Ni during the hydrogen reduction. As a result of hydrogen reduction, the porosity increase was clearly demonstrated. The anode reduction condition, especially the reduction temperature, was found to be most critical factor influencing the anode electrical conductivity.

Kinetics of sulfuric acid decomposition over iron oxide based catalysts

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The present study was aimed at developing iron oxide based catalysts for sulfuric acid decomposition that can operate in extreme conditions as posed in the actual reactor conditions. Our earlier work exhibited the efficiency of chromium doped iron oxide [1] and copper ferrite as catalysts [2] for sulfuric acid decomposition in flow through quartz catalytic reactor. In this work iron oxide and chromium doped iron oxide catalysts were prepared by co precipitation method and their catalytic performance for sulfuric acid decomposition was evaluated in absence of any nitrogen flow as diluents for more than 100 hours at 800°C. The experiments were performed in a dual tube quartz catalytic reactor which served as an integrated boiler, superheater and decomposer. The 100 h catalytic experiments were carried out with 20 gm of 3-4 mm beads of oxides and at an acid flux of 0.6 ml min^{-1}. No decrease in catalytic activity was observed during this long term experiments for both the samples, although the doped sample exhibited slightly higher catalytic activity throughout. The catalytic activities were also monitored as a function of temperature where we found that the chromium-doped sample showed much higher intrinsic activity at lower temperatures (< 775 °C) although at higher temperatures (~ 800 °C) the SO_2 yield were comparable. The effect of sulfuric acid flux on the product yield was also investigated at flow rates of 0.2-10 ml/min of sulfuric acid. Subsequently, the spent catalyst sample was analyzed ex-situ by physicochemical and spectroscopic techniques to understand the reaction mechanism and investigate any deactivation phenomenon which might be occurring at the molecular level. From the ex-situ analysis of the spent catalyst samples the most probable mechanism of the high temperature sulfuric acid decomposition reaction was proposed, which involves metal sulfate formation and then decomposition followed with an oxygen evolution step.

[1] A.M. Banerjee, M.R. Pai, K. Bhattacharya, A.K. Tripathi, V.S. Kamble, S.R. Bharadwaj, S.K. Kulshreshtha, Int. J.Hydrogen Energ. 33 (2008) 319-326.

[2] A.M. Banerjee, M.R. Pai, S.S. Meena, A.K. Tripathi, S.R. Bharadwaj Int. J. Hydrogen Energ. 36 (2011) 4768-4780.

The Management of Water in a Fuel Cell with Membrane Exchanger of Protons (PEMFC)

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Abstract:

The production of water is one of the results of the electrochemical reaction, which makes it possible to say that the management of water is essential for an ideal operation of a fuel cell PEMFC. Because a lack of water can entrained a draining of the membrane leading to the destruction of the pile, conversely, a water excess will obstruct the transport of the species present in the heart of the fuel cell, and that causes the reduction of the output of the fuel cell. Thus, we modeled the phenomenon of transport of water with various values of gradient of pressure. The simulations carried out with a simulation code of FORTRAN 6.6, the results obtained give the profiles of concentration of water through the thickness of the heart of the PEMFC to different values from the gradient of pressure.

Keywords : Fuel cell, PEMFC, Membrane, Management of water.

Hydrogen sorption kinetics of MgH_2 doped with Pd and V particles performed by mechanical milling

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Magnesium and magnesium-based alloys are promising candidates for hydrogen storage material used for energy application. They have high hydrogen storage capacity of 7.6 wt.% and low weight which makes it a strong candidate for commercial applications. However, pure magnesium hydride shows slow sorption kinetics and to improve it, different methods of synthesis have been investigated, for example additions of various catalysts and ball milled materials. The aim of this work was to study the sorption and desorption kinetics and storage capacity of hydrogen in magnesium alloys (MgH_2-Pd and MgH_2-V). The alloys have been produced by reactive mechanical milling for 24 h and 300 rpm using a planetary milling under a hydrogen atmosphere. In this work the effects of Pd and V addition were investigated on ball-milled magnesium alloys. Prior to and after hydriding, the samples were analyzed by means of X-ray diffraction (XRD), scanning electronic microscopy (SEM) and differential scanning calorimeter (DSC). The absorption and desorption kinetics were analyzed using a Sievert's apparatus. It was observed that the addition of palladium and vanadium improves the hydrogen absorption/desorption kinetics. The MgH_2-3wt.%V composite developed showed hydrogen maximum storage capacity equal to 5.3 wt. % and reaches 4 wt.% in less than 5 minutes at 300 °C. The H-storage capacity obtained for MgH_2-0.2wt.%Pd was 6.1 wt.%, while the samples with more Pd (1 and 10%) absorbed 5.3 wt.% of H_2 at 350 °C.

Radiolytic processes of hydrogen formation from n-C_6H_{14}+H_2O mixture

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Radiolytic processes of hydrogen formation from n-C_6H_{14}+H_2O mixture being of interest in the field of transformation radiation and thermal components of nuclear energy into the energy of universal energy carrier - hydrogen has been investigated. In the given work kinetics of molecular hydrogen accumulation during radiolysis of systems C_6H_{14}+H_2O and catalyst + C_6H_{14}+H_2O with different proportions and hydrocarbon-polluted waters of oil production was studied. Irradiation of ampoules with samples was carried out on isotope source of γ-quantum ^{60}Co. Source dosimetry was carried out by chemical methods – ferrasulphate, hexane. It has been established that during radiolysis of C_6H_{14}+H_2O model mixture depending upon the proportion of the components energy transfers from water to hydrocarbons and interaction of intermediate active radiolysis products with initial molecules takes place, which leads to increase of radiation chemical yield of molecular hydrogen in comparison with additive sum of yields of separate components of given systems. The dependence of $G(H_2)=f(C_6H_{14})$ has extreme character and maximum corresponds to the actual range of C_6H_{14} concentration ≈ 30-50 weight %.

For acceleration of radiolytic decomposition processes of C_6H_{14}+H_2O mixture γ-Al_2O_3 is used as catalyst. It has been discovered that Al_2O_3 accelerates the process of molecular hydrogen formation, by increasing yield from 4,5 at 296K up to 25molecules/100ev at 673K.

Hydrogen formation from hydrocarbon-polluted water systems is more expedient in practice. That's why kinetics of hydrogen formation during radiolytic decomposition of oil-polluted water systems has been investigated. It's established that radiolytic decomposition processes of water+hydrocarbon pollution systems lead to obtaining universal energy carrier with yields $G(H_2)\geq$30molecules/100ev.

In order to explain the obtained experimental data and to reveal possible mechanisms of the reactions upon radiolysis of water, hexane and water-hexane mixture modelling of the processes occuring in these systems has been carried out. Here in the following factors were taken into account: dose rate, volume of the irradiated system, time of irradiation, concentrations of components, constants of the reactions rates, etc. Modelling of the processes kinetics has been made with an aid of the program GEPASI 3 for the operational system Windows. Modelling of radiolysis of water-hexane mixture has been carried out taking into consideration slight solubility of water in hexane and vice versa. That is why the assumption was made that radiolysis of this system is similar with radiolysis of each of the components in separate. However, taking into account a possibility of diffusion of the radiolysis primary products from one phase into another, several new reactions, in comparison with modelling of water and hexane radiolysis, with the respective rate constants were added. The obtained data were compared with the experimental data at the same volume ratio of components. The comparison shows quite a good coincidence of the results that may serve as an evidence of correctness of the made assumptions.

So radiolytic processes in n-C_6H_{14}+H_2O system allow transforming radiation and thermal components of nuclear energy into the energy of universal energy carrier-hydrogen on the one hand, and promote to solve ecological problems of purification sewage waters of oil production on the other hand. Radiolysis of water-n-hexane mixed fluid in regard to radiolysis of the components passes with the great yield of molecular hydrogen. That is why radiochemical processes in hydrocarbon-polluted waters may be used for getting hydrogen.

Keywords: hydrogen, water, hexane, clean energy, radiochemical yield, mathematical modelling.

Electron Screening in Metals

J. Gajević, M. Lipoglavšek

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Low energy fusion reactions rates are enhanced very much when the reaction occurs in a metallic environment. The enhancement is described by a screening energy and depends strongly on the host material. The mechanism of enhancement is not yet fully understood. Electron screening is studied with hydrogen in metals. Large electron screening is observed when the metallic targets are put under tensile stress, either from deformation caused by hydrogen loading or from mechanical stretching. Ion implanted targets always show large electron screening, while targets prepared by absorption from gas phase show large electron screening only when they are put under tensile stress. This could be explained by moving of protons from interstitial to displaced interstitial sites in the crystal. This hypothesis will be tested by measuring cross sections in different metals and at different mechanical stresses. Interaction between protons and metallic valence electrons will be studied by measuring proton Knight shift in nuclear magnetic resonance.

CONCEPTUAL DESIGN MODEL OF THE SULFUR-IODINE S-I THERMOCHEMICAL WATER SPLITTING PROCESS FOR HYDROGEN PRODUCTION USING NUCLEAR HEAT SOURCE

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ABSTRACT

Hydrogen is the most indicated candidate for its implementation as energy carrier in a future sustainable scenario. The current hydrogen production is based on fossils fuels; they have a huge contribution to the atmosphere pollution. Thermochemical water-splitting cycles do not have this issue because they use solar or nuclear heat; their environment impact is smaller than conventional fuels. The software based on chemical process simulation (CPS) can be used to simulate the thermochemical water splitting cycle Sulfur-Iodine for hydrogen production. In the paper is developed a model for Sulfur-Iodine process in order to analyze his sensibility and calculate the efficiency and the influence of many parameters on this value.

Key Words: Thermochemical water splitting cycles, thermal efficiency, sulfur-iodine.

In-situ determination of aging precipitation in deformed Fe-Cu and Fe-Cu-B-N alloys by time resolved small-angle neutron scattering

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Abstract:

Recently it has been recognized that the precipitation of Cu nanoclusters in steels is very sensitive to the presence of (1) defect structures and (2) mobile atoms, such as B and N. Both factors play an essential role in the newly discovered self healing phenomenon in which deformation or radiation damage in steel can be repaired by precipitation of Cu and/or BN during use at high temperatures. In order to study this process in detail we have performed in-situ small-angle neutron scattering (SANS) measurements on copper precipitation in deformed Fe-Cu-B-N alloys 550 °C, combined with mechanical tests, transmission electron microscope (TEM) observations and positron annihilation spectroscopy. The results prove that copper precipitates either as spherical nanoclusters or segregates at dislocations and/or interfaces. Increasing levels of deformation promotes segregation at dislocations. The addition of boron and nitrogen accelerates the formation of spherical nanoclusters, but suppresses the Cu precipitation along dislocations in strained samples. Self healing of small defects in Fe-Cu-B-N alloys will initially take place by the formation of BN precipitates or B / N clusters, while larger defects are filled by Cu precipitates. Self healing of defects is expected to significantly extend the life time of steel components for high temperature applications in which deformation or radiation damage slowly accumulates until failure.

Keywords: *small-angle neutron scattering; Fe-Cu; Fe-Cu-B-N; self healing; precipitation kinetics; open volume defects*

FEASIBILITY OF LARGE SCALE PRODUCTION AND UTILIZATION OF HYDROGEN FUEL IN SUB-SAHARAN AFRICA

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ABSTRACT

Developing countries have abundant renewable energy resources including solar energy, wind power, geothermal energy, hydro energy and biomass, as well as the potential to manufacture adequate systems that harness these. This paper reviews the feasibility of large scale production and utilization of hydrogen fuel in Sub-Saharan Africa by actually highlighting the technicalities involved which at present is quite advanced for some of these countries. As it stands, a hydrogen economy holds a bright and promising future for developing countries but is faced with challenges that need immediate attention which are technological and political barriers, infrastructural and social– cultural issues, economic problems etc. Globally, hydrogen production is 48% from natural gas, 30% from oil, and 18% from coal. All these production routes have side effects to the environment. This review highlights the use of water splitting technologies which are attractive and environmentally favorable but account for only 4% of global hydrogen fuel production. Ways and technologies for effective storage of hydrogen as a fuel as well as the advantages, disadvantages and utilization are also documented in this paper. For a working hydrogen economy, there is need for development of the necessary infrastructure to support research, development and demonstration projects with active collaboration and financial support from developed countries. Sub-Saharan African countries should therefore have at least good labor intensive system, properly enlighten the public, create a good state-private partnership, and also implement appropriate policies so as to attain a full hydrogen economy.

Keywords: Hydrogen, Developing countries, Nigeria, Fossil fuels, Economy, Environment

Investigating the improvements in hydrogenation properties of Mg films by Ti/ Zr layer addition using NRA and ERDA

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Hydrogen storage materials have attracted world-wide attraction for increasing demands of energy for environmental protection. Among these, Mg is considered as a promising hydrogen storage material due to its high storage capacity (7.6wt %), light weight and low cost. However, thermodynamics indicate that hydrogen desorption from bulk MgH_2 only takes place at temperature above 600K, which restricts its use in practical applications, especially as hydrogen storage material in mobile applications and fuel cells which need to operate at moderate temperature and under hydrogen pressure of few bars.

Hydrogen in thin films provides an opportunity to examine a number of unusual properties, which are not present in the bulk systems, as the hydrogen adsorption, absorption and storage is basically a surface phenomena. Recently, various attempts have been undertaken to study Mg based nano composite films, mainly involving alloying Mg with other elements such as MgTi and MgNi or doping with catalysts Nb and Pd. The interest in Mg films also stems from its switchable mirror behavior which could transfer from a high reflecting state to a transparent state during hydrogen absorption.

In the present work Mg, Mg-Zr and Mg-Ti thin films sandwiched between Pd were prepared on Si substrate by vapor deposition technique at 10^{-6} torr vacuum in a chamber equipped with both electron gun and resistive heating for sequential deposition. Structural and morphological characterizations were performed using Grazing Incidence X-ray Diffraction (GI-XRD) and Atomic Force Microscopy (AFM). Hydrogenation of the films was carried out at 150°C under H_2 pressure of 1.5bar in a SS chamber for 2hrs. The chamber was pumped down to 10^{-5} torr before introducing hydrogen to it. The variation in the hydrogen content and depth distribution of Mg films upon introducing Ti/ Zr layers has been studied using Elastic Recoil Detection Analysis (ERDA) and Nuclear Reaction Analysis (NRA).

References

1. L.Z. Ouyang, H. Wang, C. Y. Chung, J. H. Ahn, M. Zhu, J. Alloys & Compounds 422 (2006) 58-61.
2. L. Pranevicius, E. Wirth, D. Milcius, M. Lelis, L.L. Pranevicius, A. Kanapickas, Surface & Coating Technology 203 (2009) 998-1003.

Hydrogen storage properties of MgH_2 alloys produced by high energy ball milling

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Among the metal hydrides, magnesium is considered as one of potential hydrogen storage materials because of its high capacity (7.6 wt%), lightweight and low cost. However, high work temperature, slow reaction kinetics and hard activation process limit the practical application of Mg-based hydrides. Recently, the reactive ball milling was successfully introduced to prepare hydrogen storage materials. In this work, MgH_2 catalyzed with Ni nanoparticle was synthesized by high pressure reactive milling under hydrogen up to 100 bar. As the results, it was found that the hydrogen absorption/desorption kinetics are stable upon cycling and far superior to nanocrystalline magnesium hydride. The absorption conditions have been found to be quite modest at 300 °C and 5.5 wt.% is reached within 5 min. Desorption into 1 bar hydrogen can be achieved at 350°C within a few minutes. The metallic Ni in nanometer scale acts as a catalyst for improvement the kinetics of MgH_2 for hydrogen storage material and at the same time allowed to reduce the milling process for short time, only 2 hours.

Kinetics of gas desorption from highly defected material

G. N. Lazareva, N. P. Lazarev

The processes of accumulation and rearrangement of gases have a substantial effect on the development behavior of the radiation damage of construction materials in nuclear reactors [1]. Helium is the major gas component which is produced during nuclear reactions in nuclear fission reactors [2], while in fusion reactors the evident problem is hydrogen and its isotopes. It is much harder to describe the behavior of gas components when high concentrations of different gases are simultaneously inserted in a material which is characteristic for all the existing reactors.

The problems of gas desorption are usually considered in the following formulation [3]. The gas atoms are able to diffuse comparatively fast with the certain diffusion coefficient D in the defect-free crystal. There are point and extended defects (vacancies, dislocations, grain boundaries, precipitations of new phases, etc.) in the bulk which can trap the gas atoms due to the positive binding energy E_b^k between the gas atom and the k-type defect. In other words, the crystal defects are traps for a gas and their strength is determined from the solution of a separate problem of attaining equilibrium distribution of gas atoms in the vicinity of a certain trap resulting from the balance of gas atoms absorbed and emitted from this trap.

The volume fraction of traps is assumed to be small in the mentioned type of approaches. The system separation on the defect-free region and the traps loses its sense in the case of highly defected crystals and especially amorphous alloys. The theory of the diffusion processes in disordered structures is applied for the solution of this problem [4]. The master kinetic equations of the hopping diffusion and the methods of their solution are formulated. The expressions for diffusion coefficients are found in the approximation which is the refinement of the one previously obtained in phenomenological approach [5]. The kinetics of gas desorption during heating linear in temperature is studied based on kinetic balance equations. The locations of maxima of gas desorption are established as well as the efficiency of absorption by various defects in the material.

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SUBSTRATE EFFECTS ON FORMATION AND HYDROGENATION OF MG-NI FILMS

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ABSTRACT

Usually thin metallic films for metal hydrides research applications are synthesised on hard and flat substrates such as silicon, magnesium oxide, fused silica or quartz glass. And in most cases they are chosen by physical properties such as surface roughness or crystal orientation. However, chemical properties of the substrate can be equally important. In this work manipulation of thin film-substrate interaction zone, modyfication of free surface energy and its effects on hydrogenation properties of thin films deposited by magnetron sputtering were analysed. For the experiments Mg_2Ni alloy and its coresponding Mg_2NiH_4 hydride were used. These materials were chosen for several reasons. First of all, since its discovery by Reilly and Wiswall in 1968 Mg_2Ni_4 became a target for many studies, therefore there are a lot of information on this hydride at different literature sources. It was revealed that in powder form Mg_2NiH_4 has three crystal phases: LT-1 and LT-2 are both monoclinic low temperature (below 510 K) phases respectively without and with microtwinings, and HT is FCC non-conducting high temperature (above 510 K) phase. For Mg_2NiH_4 powders, phase transition between low temperature and high temperature phases is reversible. On the other hand, it was shown that Mg_2NiH_4 in thin film form on quartz and calcium fluorite substrates does not undergo any phase transitions and always stays at some intermediate pseudo cubic phase. Furthermore, extensive studies have demonstrated that both for powders and thin film material crystallographic, electrical and optical properties of Mg_2NiH_4 hydride strongly depend on residual stresses as well as contaminants. These facts makes magnesium nickel hydride very attractive candidate for investigations of new approach for bulk hydride properties modification just by modifying film-substrate interaction forces. The experimental results for "soft" low surface energy teflon substrates are compared to films deposited on pure silica films with and without plasma pretreatment. It is observed that different interface zone between substrate and film has great affect on both film crystallinity and its reaction with hydrogen. It is also demonstrated that modifying substrate surface has crucial affect on film microstructure before and after hydrogenation. Metallic films were tested for hydrogen adsorbtion - desorbtion cycling and arising differences in film microstructure were revealed by scanning electron microscopy. Several physical insights and basic theoretical models for the received results are also provided.

Keywords: Hydrogen energy, hydrogen storage, metal hydride, film, substrate, plasma treatment

ANN-based prediction of a 20 kWp grid-connected photovoltaic power at Trieste (Italy)

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Abstract
Growing of PV for electricity generation is one of the highest in the field of the renewable energies and this tendency is expected to continue in the next years. Due to the various seasonal, hourly and daily changes in climate, it is relatively difficult to find a suitable analytic model for predicting the performance of a grid-connected photovoltaic (GCPV) plant. In this paper, an artificial neural network is used for modelling and predicting the power produced by a 20 kWp GCPV plant installed on the roof top of the municipality of Trieste (latitude 45_400N, longitude 13_460E), Italy. An experimental database of climate (irradiance and air temperature) and electrical (power delivered to the grid) data from January 29th to May 25th 2009 has been used. Two ANN models have been developed and implemented on experimental climate and electrical data. The first one is a multivariate model based on the solar irradiance and the air temperature, while the second one is an univariate model which uses as input parameter only the solar irradiance. A database of 3437 patterns has been divided into two sets: the first (2989 patterns) is used for training the different ANN models, while the second (459 patterns) is used for testing and validating the proposed ANN models. Prediction performance measures such as correlation coefficient (r) and mean bias error (MBE) are presented. The results show that good effectiveness is obtained between the measured and predicted power produced by the 20 kWp GCPV plant. In fact, the found correlation coefficient is in the range 98–99%, while the mean bias error varies between 3.1% and 5.4%.

Study on Solar Thermoelectric Hydrogen Energy System

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Short abstract

Solar thermoelectric power generation is attracting research at micro and macro level capacity. Hydrogen generation through solar and electrolysis is green and clean energy conversion. The components of solar thermoelectric hydrogen energy system are reviewed in this work. The solar energy is converted into hydrogen through solar energy capturing device, thermoelectric power generator and electrolysis. The solar energy capturing device is capture the solar radiation and converted into thermal energy in heat source. Thermoelectric generator is attached between heat source and heat sink and electricity is generated through seebeck effect. Generated electricity is driving the electrolysis device to generate hydrogen energy. The different solar thermoelectric hydrogen energy systems are proposed.

Keywords: Electrolysis, Solar Collector, Thermoelectric power generator

$CoTiO_3$-TiO_2 thin films prepared by Crossed Beam Pulsed Laser Deposition for hydrogen production by electrolysis.

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ABSTRACT

In the search of bifuncional fuel cell materials, $CoTiO_3$-TiO_2 thin films were obtained on glass substrates by Crossed Beam Pulsed Laser Deposition (CBPLD). Two crossed plasmas were produced by ablating simultaneously TiO_2 and Co targets. In order to vary the Co content in the films, the average kinetic energy of Co ions (E_{Co}), in the Co plasma, was changed keeping the same TiO_2 plasma conditions. The composition of the films was analyzed by Rutherford Backscattering Spectroscopy (RBS) and X-Ray Photoelectron Spectroscopy (XPS) techniques whilst the film structure was studied by Raman Spectroscopy. The optical properties were determined using the Kubelka-Munk model, from UV-Vis Spectroscopy in the reflectance mode. The electrical properties were calculated from measurements with the four-point technique. The electrochemical performance for the Oxygen Evolution Reaction (OER) was studied by cyclic and lineal voltamperometry in a standard three electrode cell of 100 cm^3, the counter-electrode was a platinum grid and as reference a Hg/Hg_2SO_4/KOH 0.5M electrode was used. The obtained composition values showed an increase of the Co content from 1.3 to 5.2 at % as the E_{Co} increased from 36 to 789 eV. Raman analysis of the thin films showed the presence of TiO_2 in its Rutile phase and the formation of $CoTiO_3$. The optical properties showed band gap values as low as 2.0 eV for the film with the highest Co content. The electrical resistivity of the deposited materials was varied from 7×10^{-1} to 1.2×10^{-3} ohm-cm, depending on the Co content, revealing the formation of a conductive material. Preliminary results of the electrochemical behavior of the films for the OER in 0.5M of KOH produced a current density around 8.3 mA/cm^2 for 1.4 V vs NHE at 23 °C and 767.1 mbar (0.75 atm) pressure, suggesting that $CoTiO_3$-TiO_2 thin films are good candidates for the oxygen evolution reaction.

Hydride formation and effects of hydrogen on the mechanical properties of Zirconium rich alloys

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Zircaloys are zirconium-based alloys extensively used as cladding materials on nuclear reactors, mainly because of its high corrosion resistance, low neutron absorption capacity and good mechanical properties at high temperatures. Due to the critical conditions of PWR reactor operation, such as high pressure (160 atm) and high temperature (320°C), these alloys undergo a process of corrosion and hydrogen produced in this reaction can be absorbed by the tube compromising their mechanical properties due to formation hydride.

The goal is to study the interaction of hydrogen with the microstructure of zirconium alloys developed for this application and compared with commercial alloys which composition are Zr-1Nb e Zr-1Nb-1Sn-0,1Fe.

Basically, the alloys were charged with hydrogen and submitted to tensile tests to evaluate the change in the mechanical properties after hydrogen charging at the typical operating temperature of nuclear reactors.

The degradation of the mechanical properties was observed after hydrogen charging due to hydride formation. It was observed a reduction in ductility after undergoing loading gaseous hydrogen (the test performed for 96h leads to a drastic reduction in ductility) and the distribution and orientation of hydrides strongly influence the fracture mechanism of hydrogenation for each condition. The same behavior is observed in Zr based alloys developed to these applications.

Novel device for simultaneous volumetric and X-rays diffraction measurements on metal-hydrogen systems

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In order to characterize and improve hydrogen storage materials in systems where many phases can be formed, it is very helpful to be able to correlate hydrogen intake with a precise determination of the hydride phases involved in the process. The aim of this work is to present a simple, compact and low cost device that performs simultaneous X-ray diffraction and hydrogen sorption measurements. The small-size reactor chamber can stand up to 6000 kPa of internal pressure while the sample can be heated up to 450ºC in vacuum or hydrogen atmosphere, and can be mounted in the sample holder space of our X-rays diffractometer. The design process was assisted by finite elements modeling and by the use of mock-up prototypes in order to optimize thermal and under-load behaviors. The acquisition and control software was designed to perform simultaneous control and measurement of volumetric and X-rays diffraction parameters (reactor inner pressure, sample temperature, in/out hydrogen flow, goniometer position, step size, integration time and detected counts). Examples of phase identification using this new device during pressure-composition isotherms and thermal desorption spectroscopy are also presented.

OVERVIEW OF HYDROGEN ECONOMY R&D ACTIVITIES IN MALAYSIA

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Abstract:

On 4 May 2010, the Government of Malaysia agreed in principle of its go-ahead for the setting up of Malaysia's first nuclear power plant (NPP) slated to operate by the year 2021. It was also hinted that only commercially proven reactors are to be considered. While this is understandable, hydrogen-lobbyists are instead hoping for Malaysia to invest in Generation IV reactors for strategic purposes i.e. generating electricity and splitting free hydrogen simultaneously. Together with current hydrogen production via steam reforming of natural gas in the oil, gas and petrochemical industries, Generation IV power reactor may help Malaysia towards realizing hydrogen as a viable alternative fuel option in the future.

While having "hydrogen-friendly NPP" helps, continuous R&D efforts are still very important. This ensures continuous generation of knowledge and improvement of technology in every aspect of the hydrogen economy. In Malaysia, hydrogen energy research group works on fuel processing, solar hydrogen and bio-hydrogen, while fuel cell research group focuses on proton exchange membrane fuel cell (PEMFC) materials such as alternative electrolyte membranes, low Pt electrodes and bipolar plates. In fact, Malaysia recently signed an agreement with IAEA to jointly study the hydrogen membrane fuel cell to encourage more R&D projects in this field. In addition, several projects are also under-going using techniques such as small angle neutron scattering (SANS) and neutron radiography at the 1-MW TRIGA Mark-II research reactor.

This poster will highlight some of the R&D and educational activities towards establishing hydrogen as a viable alternative fuel option in Malaysia.

***Keywords**: hydrogen economy; Malaysia*

A QUANTIZATION OF BOSONIC STRING

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Abstract

Bosonic string theory considers all particles as bosons, while retaining properties such as the absence of fermions. Physicists have calculated that for consistency, bosonic string theory requires 26 dimensions and space. This quantization occurs analogously to the quantization performed for a scalar field in quantum field theory.

Introduction

For the quantization of a string exploit diverse knowledge of classical and quantum physics, essentially the three pillars of quantization are the branches of quantum mechanics, special relativity and Lagrangian mechanics, all applied to the concept of field. These skills range from simple concepts such as an inertial reference frame, Lorentz transformations, through the very practical light cone coordinates, to concepts like Feynman integrals, gauge fields, the action of Nambu-Goto and the Polyakov , Moduli spaces, Riemann surfaces and culminating with the famous Veneziano amplitude.

Methodological design

The proposed methodology of this study is based on the literature review on the issues involved for both mathematical and physical understanding the quantization of a bosonic string. These themes are developed in an original, so that written language was used to explain simple concepts, while not complicated, the relationship between them can be complex.

Since it can be shown that the string is a system that has ties can proceed to quantize following two options:

- Quantize the theory without taking into account the bonds. Then define operators of the bonds and find states that are annihilated by them.

- Resolve ties to classical level and then quantize the system on the reduced phase space (which is consistent with the bands).

The first case is a covariant canonical quantization and the second case the light cone quantization. There is a third possibility of quantization, using the path integral. For simplicity, take the light cone quantization.

Conclusions

1. On the quantization of bosonic string, to be mathematically consistent, it is necessary to

consider a space of 26 dimensions, of which 25 are spatial and temporal.

2. The light cone coordinates simplify the quantization enough rope for both the case of the open string and closed string.

3. The Euler-Lagrange equations optimize a functional and widely used also in string theory.

4. Gravitation is a natural consequence of string theory.

5. Photons, which are particles of the electromagnetic field appear in the quantization of open string.

6. Gravitons, which are the quanta of the gravitational field appear in the quantization of closed string.

7. Schrodinger equation applied to the states of the quantization of open bosonic string turns out to be equivalent to the Maxwell equations for the electromagnetic field.

8. World sheets in the interactions between strings are perfectly represented by Riemann surfaces.

9. All particles representing the known interactions may appear in the quantization of bosonic string.

10. Veneziano amplitude, considered as the beginning of the string theory can be explained and motivated in a natural way using Riemann surfaces.

11. The quantization of bosonic string is analogous to the covariant quantization in quantum field theory.

12. Be seen to string theory as an excellent candidate for unified theory.