

**Report on the Second International Symposium on Hydrogen in Matter
(ISOHIM 2005)**

Ångström laboratory, Uppsala University, Uppsala, Sweden

June 13-17, 2005

S p o n s o r s:

The Royal Swedish Academy of Sciences, ESF Programme Psi-k, The Swedish Research Council, US Department of Energy, The Swedish Energy Agency, NIST, NASA/JPL, Argonne National Laboratory, Jefferson Lab, Uppsala University, City of Uppsala, as well as industrial companies, the Reference Metals Company, Inc. and ATI Wah Chang.

O r g a n i z e r s:

ISOHIM BOARD MEMBERS are Jim Miller (Chair, ANL, USA), Ganapati Rao Myneni (Co-Chair, JLAB, USA), Björgvin Hjörvarsson (Co-Chair, Uppsala University, Sweden), Gunter Luepke (Secretary, College of W&M, USA), Bob Bowman (JPL, Caltech, USA), Tadeu Carneiro (Reference Metals, USA), Christian Day (FZK, Germany), Ron Graham (Wahchang, USA), Bill Lanford (UNY Albany, USA), Peter Lindblad (Uppsala University, Sweden), and Matthew McCluskey (WSU, USA Richard Ricker, NIST, USA).

The LOCAL ORGANIZING COMMITTEE included:

I. Abrikosov, Y. Andersson, C. Chakon, O. Eriksson, K. Flodström, B. Hjörvarsson, E. B. Karlsson, P. Lindblad, and L. Westerberg

<http://www-conference.slu.se/ISOHIM/index.htm>

The Second International Symposium on Hydrogen in Matter was held June 13-17, 2005 at the Ångström laboratory, Uppsala University, in Uppsala, Sweden. The mission of ISOHIM 2005 was to advance the basic understanding of hydrogen-matter interactions. ISOHIM operates on an international level, promoting worldwide information exchange and collaboration. The interdisciplinary nature of the conference is easily recognized. It ranges from hydrogen induced embrittlement in construction materials to quantum correlations in biological systems. It is therefore of uttermost importance to link the experimental and the theoretical efforts to obtain better understanding within the field of hydrogen in matter.

Surfaces, interfaces as well as defects play a major role for chemical affinity and fugacity as seen e.g. by the catalytic activity and selective reaction paths of designed surfaces and interfaces. The composition, structure and extension are all important, nevertheless finite size effects are only rarely discussed in this context. The quantum nature of the electronic building blocks

is the fundamental entity, which can never be ignored. This is one of the main missions of the conference. As an example the photobiological activity of surfaces was mentioned. Finite size effects are apparently important for the reactivity, as well as the geometrical factors of the surfaces. This was treated in a session where we linked together specialists from different disciplines, with the aim of enlightening the field by cross disciplinary discussions.

Meeting Programme was directed to the following 6 main topics:

Fundamentals: Dynamics and thermodynamics of H in metals, semiconductors and oxides. Quantum effects. Hydrogen surface and interface interactions, Defects & doping

Hydrogen induced modifications of materials: Optical and electric properties of materials, Magnetic properties of materials, Mechanical properties of materials

Biological aspects: Hydrogen production using biological processes, Artificial photosynthesis, Other aspects

Technological aspects: Ultra pure materials, UHV applications, Alloy production, Powder production, Nuclear reactors

Energy related aspects: Hydrogen storage and purification, Energy conversion Fusion technology

New aspects

The conference attracted 95 participants from 18 countries. There were 19 plenary/invited and 33 contributed talks presented, as well as 28 poster presentations. On Friday, June 17, a Panel Discussion was organized, and most important directions of hydrogen related research in the future were discussed. The Psi-k community was well represented, e.g. we have organized a session at the conference with Invited Talk given by G. Brocks (Computational Materials Science, MESA+ Research Institute, University of Twente, 7500 AE Enschede, The Netherlands) "Excitations in metal hydrides from first principles". But in addition, there were many other talks devoted to theoretical studies of hydrogen-related phenomena by means of first-principles methods of the electronic structure theory.

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Programme

Monday, June 13

17.00 - 21.00 Registration and welcome party

Tuesday, June 14

9.15-9.30 Welcome

Session Chairman B. Hjörvarsson

9.30 - 10.15 **C. Van de Walle (plenary)**, Universal alignment of hydrogen levels in semiconductors, insulators, and solutions.

10.15 - 10.45 Break

10.45 - 11.30 **B. Beck Nielsen (plenary)**, Hydrogen in group-IV semiconductors and its interaction with defects.

11.30 - 11.50 G. Lüpke, Vibrational lifetime of hydrogen bending mode in silicon.

11.50 - 12.10 Y. Oya, Hydrogen isotope behavior in helium ion pre-irradiated SiC.

12.10 - 12.30 M. I. J. Probert, Ab Initio Path Integral MD Simulation of Hydrogen in Silicon

12.30 - 14.00 Lunch

Session Chairman R. Kirchheim

14.00 - 14.30 **E. Babaev (invited)**, A superconductor to superfluid phase transition in the projected liquid metallic state of hydrogen.

14.30 - 14.50 G. Cao, H induced modifications of optical and electronic properties of Mg films

14.50 - 15.10 R.A.H. Niessen, Electrochemical hydrogen storage characteristics of thin film MgX (X = Sc, Ti, V, Cr) compounds

15.10 - 15.30 N. Patel, Thermal stability of hydrogenated Mg/Al thin films

15.30 - 15.50 D. Milcius, The role of grain boundaries in the mechanism of plasma immersion hydrogenation of nanocrystalline MgAl films

15.50 - 16.15 Break

Session Chairman E. B. Karlsson

16.15 - 16.45 **C. Rolfs (invited)**, Electronic screening in deuterated metals.

16.45 - 17.05 L. Havela, Magnetic properties of hydrides of uranium ternary intermetallics

17.05 - 17.25 P. V. Sushko, Optical absorption and electrical conductivity of H-doped $12\text{CaO} \cdot \text{X}_7\text{Al}_2\text{O}_3$

17.25 - 17.45 Rick L. Paul, Measurement of Hydrogen in Advanced Materials by Cold Neutron Prompt Gamma-ray Activation Analysis

Tuesday, June 14

Session Chairman P. Lindblad

8.45 - 9.30 **L. Hammarström (plenary)** Hydrogen from sun and water: Biomimetic approaches to artificial photosynthesis.

9.30 - 10.15 **W. Lubitz (plenary)**, The Enzyme Hydrogenase Structure and Function as Studied by Spectroscopic and Theoretical Methods.

10.15 - 10.45 Break

Session Chairman R. L. Paul

10.45 - 11.20 **S. Seetharaman (invited)**, Hydrogen in steel making.

11.20 - 11.50 D. Fruchart, Hydrogen used as a tool to probe magnetic materials: from soft and amorphous to hard and crystallised magnetic systems

11.50 - 12.10 C. Zlotea, MgH₂ whiskers formation by hydrogen disproportionation of Mg₂₄Y₅.

12.10 - 12.30 R. C. Bowman, Roles of Hydrogen in Space Explorations

12.30 - 14.00 Lunch

Session Chairman W. A. Lanford

14.00 - 14.45 **P. Sofronis (plenary)**, Mechanisms and models for hydrogen embrittlement.

14.45 - 15.05 A-M. Alvarez, Hydrogen embrittlement in a metastable β -titanium alloy

15.05 - 15.25 A. V. Golubeva, Hydrogen retention in plasma-sprayed tungsten and tungsten-rhenium alloys

15.25 - 15.45 I. P. Chernov, Excitation of hydrogen subsystem in solid by external influence

15.45 - 16.05 B. Zajec, Hydrogen permeation through a metal membrane in the recombination limited regime

16.05 - 16.30 Break

Session Chairman Y. Andersson

16.30 - 16.45 J. S. Brown, Superconducting protons in metals

16.45 - 17.00 H. Londer, New high capacity Getter for vacuum insulated mobile LH2 storage tank systems

17.00 - 19.00 **P. Poster Session**

Thursday, June 16

Session Chairman S. Seetharaman

8.45 - 9.30 **K. Abiko (plenary)**, Metallurgy to discover amazing metals - ultra-purification to develop ductile metals.

9.30 - 10.15 **W. Singer (plenary)**, High-purity niobium for superconducting radio frequency resonators.

10.15 - 10.45 Break

Session Chairman D. Fruchart

10.45 - 11.30 **R. Kirchheim (plenary)**, Interaction of hydrogen with defects and their stabilization.

11.30 - 11.50 K. Sakaki, The relation between vacancy formation and phase transformation in $\text{Pd}_x\text{Ag}_{1-x}\text{-H}$ system

11.50 - 12.10 A. Talyzin, Fragmentation of C_{60} by strong hydrogenation: a route to synthesis of new materials.

12.10 - 12.30 K.O. Kvashnina, X-ray absorption and emission study of C_{59}H_x and C_{58}H_x fullerenes

12.30 - 14.00 Lunch

Session Chairman R. C. Bowman

14.00 - 14.30 **L. Hallstadius (invited)**, Hydrogen pickup in zirconium alloys - a nuclear fuel industry perspective.

14.30 - 14.50 J. F. Miller, Lightweight materials for hydrogen storage.

14.50 - 15.10 M.H. Sørby, Characterization of mixed aluminates and the role of Ti doping.

15.10 - 15.30 O. M. Løvvik, First principles study of earth alkaline aluminates.

15.30 - 15.50 C. Moysés Araújo, Vacancy mediated hydrogen de-sorption in crystalline sodium aluminate

15.50 - 16.30 Break

Session Chairman I. Abrikosov

16.30 - 17.00 **G. Brocks (invited)**, Excitations in metal hydrides from first principles.
17.00 - 17.20 M.G. Shelyapina, First-principles investigation of the stability of the Ti-V-Cr ternary alloys and their related hydrides.
17.20 - 17.40 M.J. van Setten, Optical properties of hydrogen storage materials: a first principles approach.
17.40 - 18.00 H. Jonsson, Binding and diffusion of hydrogen in magnesium alloys.

Friday, June 17

Session Chairman L. Westerberg

8.45 - 9.30 **R. J. Reid (plenary)**, Why worry about outgassing?
9.30 - 10.15 **P. Chiggiato (plenary)**, Methods for reduction of hydrogen outgassing.

10.15 - 10.45 Break

Session Chairman H. S. Hseuh

10.45 - 11.30 **R. C. Bowman (plenary)**, Hydrogen outgassing behavior in the gas gap heat switches of the Planck sorption cooler.
11.30 - 11.50 S. Anakhov, Gas Distribution in High Purity Niobium EB Welded in UH Vacuum
11.50 - 12.30 **V. Nemanic (invited)**, Hydrogen outgassing from stainless steel - new experimental data

12.30 - 14.00 Lunch

Session Chairman R. J. Reid

14.00 - 14.30 **H. C. Hseuh (invited)**, Beam induced pressure rise in high intensity hadron machines.
14.30 - 15.00 **E. Mahner (invited)**, A review of heavy-ion induced molecular desorption studies for practical accelerators.
15.00 - 15.20 J. Wolf, Outgassing measurements with a prototype for a large XHV spectrometer.
15.20 - 15.40 J. Setina, Hydrogen outgassing of stainless steel vacuum chamber.
15.40 - 16.00 E. Hedlund, A comparison of published data on hydrogen outgassing from stainless steel

15.50 - 16.30 Break

16.30 - 17.00 **Panel discussion:** Status and where do we go next.

17.00 - 17.30 Summary, closing remarks, and rewards

Abstracts of presented papers can be requested from conference organizers.

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