Peter Kalisvaart

Post-doctoral fellow
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PhD: **Eindhoven University of Technology,** Materials Science, December 2008
M.S.: **Eindhoven University of Technology,** Chemical Engineering, October 2003

Current status: Dutch Citizen, Temporary worker in Canada.

Areas of expertise: Hydrogen storage, General materials science, Electrochemistry, Batteries, Neutron scattering techniques.

Working Experience:

Post-doctoral fellowship at the University of Alberta, Department of Chemical and Materials Engineering. *(June 2009- present)*

Current supervisor: Professor Dave Mitlin

- Performed experimental research on Mg/based hydrides and Li-ion batteries, putting everything I learned during my PhD to good use.
- Published 4 first-author papers and co-authored 14 in total.
- Developed extensive working knowledge and experience in neutron reflectometry experiments and data processing as applied to thin film energy storage materials in collaboration with the Canadian Neutron Beam Centre in Chalk River Ontario. This has resulted in 5 joint publications[1,3,5,7,13] also involving people from NIST and the Helmholz Institute in Germany.
- Co-supervise 3 graduate students, XueHai Tan, Elmira Memarzadeh and Alireza Kohandehghan.
- Maintained collaboration with the Molecular Catalysis group of Rutger van Santen at Eindhoven University of Technology. Resulted in 2 joint publications[10, 12], one of which[12] united the core competencies of both our groups, transmission electron microscopy and density functional theory calculations.

My research initially focused on Magnesium-based hydrogen storage materials. We specifically studied the effects of addition of transition metals to magnesium by sputtering (1-2 micron thick films) on the kinetics of magnesium hydride formation. I wrote an extensive overview paper on a wide range of alloy compositions, comparing their kinetic properties and comparing reactive (Mg-Al-Fe) and 'simple' Mg-catalyst composites (Mg-AlTi and Mg-FeTi)[14]. We were the first to prepare and study free-standing multilayered materials of Mg and a TM-based catalyst[6, 4] and they showed comparable performance to cosputtered alloys for the same weight% of alloying elements. We discovered that Mg/TM multilayers develop a very special morphology with the Mg forming large particles that are protected from further agglomeration by the TM layers[6].

From the start of 2012 to the present, my research focused on Si-based anodes for Li-ion batteries. We are performing a systematic study of the influence of the length and diameter of silicon nanowires as well as coating layers on their electrochemical cycling stability with a strong emphasis on post-cycling microstructural characterization[2].

Development engineer at Philips Lighting, department PDLC (Process Development Lighting Components). *(April 2008-April 2009, department no longer exists)*

- Member of a team of 'troubleshooters', solving specific problems in Philips Lightings' manufacturing facilities in The Netherlands and Belgium.
- Developed expertise in quartz glass manufacturing, specifically high-temperature corrosion of tungsten furnaces in humid gas streams.

Prior education:

PhD study on Mg-based alloys for hydrogen storage under supervision of prof. dr. P.H.L. (Peter) Notten at Eindhoven University of Technology. *(January 2004-April 2008)*

- 4 first-author publications related to PhD Thesis. Co-authored total of 9 papers.
- Obtained extensive knowledge on all aspects of electrochemistry relevant to batteries, both Ni-MH and Li-ion
- Hands-on experience performing neutron diffraction experiments at the Institut Laue Langevin in Grenoble, France
- Acquired a working knowledge of solid-state nuclear magnetic resonance

My work focused on the preparation and characterisation of Mg-TM (TM=Sc,Ti) bulk alloys and hydrides. These materials can, potentially, store 5 times as much hydrogen as present-day AB_5-type materials used in Ni-MH batteries. Alloying Mg with only 20at% of either of these two elements induces a structure change in the hydride from rutile to fluorite resulting in an 8 orders of magnitude increase in hydrogen diffusion rates. Since Scandium is prohibitively expensive, ways were found to produce metastable Mg(Ti) solid solutions by mechanical alloying.

Successful defense of the resulting PhD thesis "Preparation and Characterization of Mg-based Hydrogen Storage Materials" on December 2nd 2008. Electronic copy available from http://alexandria.tue.nl/ extra2/200910005.pdf

MS in Chemical Engineering at the Eindhoven University of Technlogy (TU/e) *(1998-2003)*

Masters thesis on luminescence properties of nanocrystalline Manganese-doped Zinc Sulphide in the group Solid-State and Materials Chemistry (SVM) of prof. dr. G. de With.

My parents' farm *(entire life)*

This made me so that I love getting my hands dirty. I also learned how to thatch roofs, a rare skill these days.

Academic network and contacts

Core Committee for PhD defence:

1. Prof. dr. Peter H.L. Notten (1st promotor, TU Eindhoven)
p.h.l.notten@tue.nl
2. Dr. H.T. (Bert) Hintzen (copromotor, TU Eindhoven)
h.t.hintzen@tue.nl
3. prof. dr. Rutger A. Van Santen (TU Eindhoven)
r.a.v.santen@tue.nl
4. Dr. Michel Latroche (CNRS, Thiais)
michel.latroche@icmpe.cnrs.fr
5. Prof. Dr. Ronald P. Griessen (VU Amsterdam, *retired*)

6. Dr. Helmut Fritzsche (Canadian Neutron Beam Center (CNBC) Chalk River, ON)
helmut.fritzsche@nrc.gc.ca
Collaboration has resulted in 5 joint publications[1, 3, 5, 7, 13] on neutron reflectometry on Mg-based thin films.

7. Dr. Pieter Magusin (Solid-State NMR expert, Eindhoven University of Technology, Eindhoven, Netherlands)
P.C.M.M.Magusin@tue.nl

Language skills:
Fluent in English and Dutch; passively fluent (reading and listening) in French and German.

Miscellaneous:
My hobbies are playing chess and cycling. I have completed the official 'Chess-trainer A' course of the Royal Dutch Chess Association (KNSB) in 2007 and instructed three advanced young players at my local chess club in Eindhoven for 3 years, prior to coming to Canada.

Appendix I: Peer-reviewed publications and conference abstracts

Full papers:

2012

1. W.P. Kalisvaart, E.J. Luber, E. Poirier, C.T. Harrower, A. Teichert, D. Wallacher, N. Grimm, R. Steitz, H. Fritzsche, D. Mitlin, *Probing the room temperature deuterium absorption kinetics in nanoscale magnesium based hydrogen storage multilayers using neutron reflectometry, X-ray diffraction, and atomic force microscopy*, Journal of Physical Chemistry C, **116**, 5868 (2012)
2. E.L. Memarzadeh, W.P. Kalisvaart, A. Kohandehghan, B. Zahiri, C.M.B. Holt, D. Mitlin, *Silicon nanowire core aluminum shell coaxial nanocomposites for lithium ion battery anodes grown with and without a TiN interlayer*, Journal of Materials Chemistry, **22**, 6655 (2012)
3. H. Fritzsche, W.P. Kalisvaart, B. Zahiri, R. Flacau, D. Mitlin, *An in-situ neutron reflectometry study of the deuterium absorption and desorption of Mg thin films alloyed with Fe and Cr*, International Journal of Hydrogen Energy, **37**, 3540 (2012)
4. R. Zahiri, B. Zahiri, A. Kubis, W.P. Kalisvaart, B. Shalchi Amirkhiz, D. Mitlin, *Microstructural evolution during low temperature sorption cycling of Mg-AlTi multilayer nanocomposites*, International Journal of Hydrogen Energy, **37**, 4215 (2012)

2011

5. W.P. Kalisvaart, E. J. Luber, H. Fritzsche, D. Mitlin, *Effect of alloying with chromium and vanadium on hydrogenation kinetics studied with neutron reflectometry*, Chemical Communications, **47**, 4294 (2011)
6. W.P. Kalisvaart, A. Kubis, B.S. Amirkhiz, D. Mitlin, Microstructural evolution during hydrogen sorption cycling of Mg-FeTi nanolayered composites, Acta Materialia, **59**, 2083 (2011)
7. E. Poirier, C.T. Harrower, W.P. Kalisvaart, A. Bird, A. Teichert, D. Wallacher, N. Grimm, R. Steitz, D. Mitlin, H. Fritzsche, *Deuteration of $Mg_{70}Al_{30}$ thin films with bilayer catalysts: a comparative neutron reflectometry study*, Journal of Alloys and Compounds, **59**, 5466 (2011)
8. B.S. Amirkhiz, B. Zahiri, W.P. Kalisvaart, D. Mitlin, *Synergy of elemental Fe and Ti promoting low temperature hydrogen sorption cycling of Mg*, International Journal of Hydrogen Energy, **36**, 6711 (2011)
9. L. Zhang, C.M.B. Holt, E.J. Luber, B.C. Olsen, H. Wang, M. Danaie, X. Cui, X. Tan, V.W. Lui, W.P. Kalisvaart, D. Mitlin, *High rate electrochemical capacitors from three-dimensional arrays of vanadium nitride functionalized carbon nanotubes*, Journal of Physical Chemistry C, **115**, 24381 (2011)
10. S.X. Tao, W.P. Kalisvaart, M. Danaie, D. Miltin, P.H.L. Notten, R.A. van Santen, and A.P.J. Jansen, *First principle study of hydrogen diffusion in equilibrium rutile, rutile with deformation twins and fluorite polymorph of Mg hydride,* International Journal of Hydrogen Energy, **36,** 11802 (2011)
11. X. Tan, M. Danaie, W.P. Kalisvaart, D. Mitlin, *The influence of Cu substitution on the hydrogen sorption properties of magnesium rich Mg-Ni films*, **36**, 2154 (2011)

2010

12. M. Danaie, S.X. Tao, W.P. Kalisvaart, D. Mitlin, *Analysis of deformation twins and the partially dehydrogenated microstructure in nanocrystalline magnesium hydride (MgH_2) powder*, Acta Materialia, **58**, 3162 (2010)
13. C.T. Harrower, E. Poirier, H. Fritzsche, W.P. Kalisvaart, S. Satija, B. Akgun, D. Mitlin, *Early deuteration steps in $Mg_{70}Al_{30}$ thin film observed at room temperature,* International Journal of Hydrogen Energy, **35**, 10343 (2010)
14. W.P. Kalisvaart, C.T. Harrower, J. Haagsma, B. Zahiri, E.J. Luber, C. Ophus, E. Poirier, H. Fritzsche, D. Mitlin, *Hydrogen storage in binary and ternary Mg-based alloys: a comprehensive experimental study,* International Journal of Hydrogen Energy, **35**, 2091 (2010)
15. S. Srinivasan, P.C.M.M. Magusin, W.P. Kalisvaart, P.H.L. Notten, F. Cuevas, M. Latroche, R.A.v. Santen, *Nanostructures of $Mg_{0.65}$ $Ti_{0.35}$ D_x studied with x-ray diffraction, neutron diffraction, and magic-angle-spinning H^2 NMR spectroscopy*, Physical Review B, **81**, 054107 (2010)

2009

16. D. Moser, D.J. Bull, T. Sato, D. Noreus, D. Kyoi, T. Sakai, N. Kitamura, H. Yusa, T. Taniguchi, W.P. Kalisvaart, P.H.L. Notten, *Structure and stability of high pressure synthesized Mg-TM hydrides (TM = Ti, Zr, Hf, V, Nb and Ta) as possible new hydrogen rich hydrides for hydrogen storage*, Journal of Materials Chemistry, **19**, 8150 (2009)

2008

17. W.P. Kalisvaart, M. Latroche, F. Cuevas, P.H.L. Notten, *In situ Neutron Diffraction study on Pd-doped $Mg_{0.65}Sc_{0.35}$ electrode material.,* Journal of Solid-State Chemistry, **181**, 1141 (2008)
18. B.R. Pauw, W.P. Kalisvaart, M.T.M. Koper, P.H.L. Notten, *Cubic MgH_2 stabilized by alloying with Transition Metals: A DFT study*, Acta Materialia, **56**, 2848 (2008)
19. P.C.M.M. Magusin, W.P. Kalisvaart, P.H.L. Notten, R.A. van Santen, *Magnesium Transition Metal alloys for hydrogen storage; Hydrogen binding sites and dynamics in MgSc hydrides*, Chemical Physics Letters, **456**, 55 (2008)
20. W.P. Kalisvaart, P.H.L. Notten, *Mechanical Alloying and hydrogen storage of Mg-based systems*, Journal of Materials Research, **23**, 2179 (2008)

2007

21. W.P. Kalisvaart, H.J. Wondergem, F. Bakker, P.H.L. Notten, *Mg-Ti based materials for electrochemical hydrogen storage*, Journal of materials research, **22**, 1640 (2007)
22. W.P. Kalisvaart, P. Vermeulen, A.V. Ledovskikh, P.H.L. Notten, *The electrochemistry and modelling of hydrogen storage materials*, Journal of Alloys and Compounds, **446-447**, 648-654 (2007)
23. M.S. Conradi, M. P. Mendenhall, T.M. Ivancic, E.A. Carl, C.D. Browning, P.H.L. Notten, W.P. Kalisvaart, P.C.M.M. Magusin, R.C. Bowman jr., S-J. Hwang, N.L. Adolphi, *NMR to determine rates of motion and structures in Metal-Hydrides*, Journal of Alloys and Compounds, **446-447**, 499-503 (2007)

2006

24. W.P. Kalisvaart, R.A.H. Niessen, P.H.L. Notten, *Electrochemical hydrogen storage in MgSc alloys: A comparative study between thin films and bulk materials*, Journal of Alloys and Compounds, **417**, 280 (2006)
25. M. Latroche, W.P. Kalisvaart, P.H.L. Notten, *Crystal structure of $Mg_{0.65}Sc_{0.35}D_x$ deuterides studied by X-Ray and Neutron powder diffraction,* Journal of Solid State Chemistry, **179**, 3024-3032 (2006)

Invited talks:

"Hydrogen Storage Materials 2012: Status and Future Prospects", W.P. Kalisvaart, D. Mitlin, *Canadian association of Physicists (CAP) Annual Congress*, Calgary Canada (2012)

"Silicon Nanowire Core Aluminum Shell Coaxial Nanocomposites for Lithium Ion Battery Anodes Grown with and without a TiN Interlayer", *TMS 2013 (accepted)*, San Antonio, USA (2013)

Conference Abstracts:

"Deuterium Absorption Kinetics in Mg-based Hydrogen Storage Materials studied with Neutron Reflectometry", *Neutrons for Energy*, Delft, The Netherlands (2012)

"Neutron reflectometry study of Magnesium Chromium Vanadium alloy spanning one complete absorption-desorption cycle", W.P. Kalisvaart, H. Fritzsche, D. Mitlin, *Hydrogen and Fuel Cells*, Vancouver Canada (2011)

"Microstructural evolution during hydrogen sorption cycling of Magnesium-TransitionMetal nanolayered composites", W.P. Kalisvaart, A. Kubis, B.S. Amirkhiz, D. Mitlin, *MRS spring meeting*, San Francisco US (2011)

"Hydrogen Storage in binary and ternary Mg-based Alloys: a comprehensive experimental Study", W.P. Kalisvaart, B. Zahiri, B.S. Amirkhiz, M. Danaie, C. Ophus, J. Haagsma, C.T. Harrower, D. Mitlin, *presented at 1st International Conference on Materials for Energy,* Karlsruhe Germany (2010)

"Mg-Ti based materials: A promising new class of high-capacity, light-weight hydrogen storage materials", W.P. Kalisvaart, P.H.L. Notten, *presented at the 58th annual ISE meeting*, Banff Canada (2007)

"Novel Mg-Ti based materials for hydrogen storage", W.P. Kalisvaart, P.H.L.Notten, *presented at the MRS fall meeting 2006,* Boston USA

"Electrochemical Hydrogen storage in $Mg_xSc_{1-x}Pd_y$ alloys", W.P. Kalisvaart, P.H.L. Notten, *presented at the 207th ECS metting*, Quebec City Canada (2005)