Energy Outlook International Institute for Carbon-Neutral Energy Research

Prospects and challenges of fuel cell vehicles

~ Navigating the rough path to a hydrogen-powered society ~

Special Interview

International Institute for Carbon-Neutral Energy Research (I²CNER), Kyushu University



TOYOTA MOTOR CORPORATION Project General Manager <u>R & D M</u>anagement Division

Katsuhiko HIROSE







KYUSHU UNIVERSITY



Petros Sofronis Toyota pre-launched the Prius back in 1997 and flooded the world markets in 2010. What are the future perspectives on the fuel cell vehicle (FCV)?

Katsuhiko Hirose We would like to make the FCV launch as successful as the Prius case, hopefully following a similar trajectory as the Prius. But unlike the time of the Prius where we had no competitors in the first 10 years and no issues of infrastructure development, we are now being chased by competitors and facing the challenge of undeveloped infrastructure. However, we regard having competitors from the beginning as an advantage, since their existence is important for creating a market.

Sofronis I like your point about the competitiveness of the

market. It would also enhance technological development and bring innovation to the field. Does Toyota have a specific timeline for the introduction of the FCV?

Hirose It will definitely be sometime in 2015 for Japan, the US, and Europe.

Sofronis I see. With regard to its development, can you share with us any technology barriers that you are facing? Further, how can I²CNER contribute to addressing those barriers?

Hirose The reason we are bringing the FCV to the market is to solve energy issues for the future. For that reason, having a long vision for the future is crucial and we need to think not only about developing technology for vehicles, like hydrogen storage and hydrogen production from renewable energy, but

Decial. Katsuhiko HIROSE Petros SOFRONIS Prospects and challenges of fuel cell vehicles

~ Navigating the rough path to a hydrogen-powered society ~

Considering that about 20% of the CO₂ emissions in Japan are generated from the transportation sector alone, there has never been a more urgent call to work toward reducing greenhouse gases than there is today. Despite its initial cost restraints, the fuel cell vehicle, first developed in 1966, holds great potential for scaling back society's dependence on fossil fuels. Hydrogen technology has rapidly evolved since then, which helps to mitigate some of the expense. However, other issues that create road blocks to the progress of the fuel cell

vehicle still need to be considered, such as infrastructure integration. What are the key challenges and crucial steps toward establishing widespread use of fuel cells and helping society advance towards a greener future?

Katsuhiko HIROSE

TOYOTA MOTOR CORPORATION Project General Manager R & D Management Division, Fuel Cell System Development Division, Energy Affairs Department

Mr. Katsuhiko Hirose obtained his first degree in physics from the School of Science and received his master's degree in Applied Physics from the Faculty of Engineering at Nagoya University, Japan. He has been an engine engineer at TOYOTA Motor Corporation since 1981, specializing in Engine, Hybrid and Emission control

technologies of vehicles. After the successful launch of the 2nd generation Prius to the US, Japan, and Europe at the end of 2003, he moved on to the new challenge of fuel

cell development. Since then, he has been working on advanced fuel cell system development, advanced hydrogen storage technologies, and hydrogen strategy. He is now responsible for hydrogen energy and infrastructure development. also the technology for implementing the new energy system into existing infrastructure. The established energy system has already reduced most of the investment costs, but we still need to put a price tag on hydrogen, which includes the cost of production, delivery, and dispensing. These aspects are often ignored by universities and institutions, but in order to influence future energy, this part is very important. I strongly recommend that I²CNER, as an institution for Carbon-Neutral Energy systems, touch on these issues.

Sofronis In order to have fuel cells on the roads, a key technology related to the transportation and dispensing of hydrogen is compressor technology. Are there any key system compressor technologies, materials, or new thermodynamic cycles that we need to investigate? Do you think this is an area in which I2CNER can invest?

Hirose The biggest barrier right now is the initial investment costs of the new system. We can take down this barrier if we find a highly efficient compressor with a lower price. Recently, we have heard evolutionary compressors rather than normal mechanical ones, such as electrochemical compressors from the I²CNER presentations and other institutes. Improving existing technology is something industry can do, so we expect innovative work from I²CNER.

Sofronis This is precisely what our mission is. We aim to pursue a type of science that has not just incremental effects on existing technology, but rather, large effects, as you've pointed out.

Hirose Are there any analytical maps that illustrate the process from the production to the consumption of hydrogen or renewable energy? This kind of analysis is necessary to identify the weak or missing point for each stage of development. The energy issue, from beginning to end, is a long sequence, so one lacking piece can be very fatal for its implementation.

Sofronis I cannot agree with you more. The road map for our institute is a dynamic process. For its creation, we communicate with all related parties such as industry, agencies like the Ministry of Economy, Trade and Industry, and the New Energy and Industrial Technology Development Organization here in Japan, or the Department of Energy in the US, to get information on how the hydrogen economy is or should be moving ahead. Soon, we will have finalized a road map, both for the Institute and the various thematic research clusters within I²CNER.

Hirose We should set aggressive targets and then create a road map to reach them. For example, if we really plan to reduce CO₂ by 80% by 2050, all necessary steps have to be well identified. For many established targets, the price of hydrogen is comparable with current gasoline or diesel, but in order to improve on a larger scale, we need a mechanism to encourage people to use hydrogen. If the price of hydrogen is the same as gasoline, no one will be willing to use it.

Informing the public about hydrogen

Sofronis Engaging the public is very important. Public understanding of new technologies is a crucial aspect of the overall discussion.

Hirose Certainly, energy being clean is not enough to convince customers. It either has to be cheap or benefit the customer in some other way.

Sofronis Yes. One of the issues that the public is always

Petros SOFRONIS

Director, International Institute for Carbon-Neutral Energy Research (I²CNER), Kyushu University

Professor, Department of Mechanical Science and Engineering, UIUC, U.S.A

Prof. Sofronis graduated from the Department of Mechanical Engineering, Aristoteleion University in Greece in 1980. He obtained his MS and PhD degrees from the Department of Theoretical and Applied Mechanics of the University of Illinois at Urbana-Champaign (UIUC) in 1983 and 1987, respectively. In 1991, he joined UIUC as a faculty member and has since been a principal investigator at the Materials Research Laboratory, playing an active role in the research field of environmental degradation of materials. He has investigated hydrogen embrittlement of materials by coupling mechanics of materials with experimental observation at the atomistic scale.

His theory on hydrogen-induced shielding of defect interactions is the



interested in when it comes to new technology is safety and reliability. Where are we today regarding harmonization of codes and standards in this regard?

Hirose Harmonization on the vehicle side is well done. The infrastructure side is not yet harmonized, as necessary safety protocols or conditions have not been discussed and agreed upon. This is mainly because refueling stations are governed by the building codes of the countries or even regions in which they are built. I do not yet have a concrete idea of how we will proceed, but we need some kind of common understanding on how to satisfy people with hydrogen. In order to do so, we need to communicate with the public. This is an element which I have noticed is missing from most research centers today.

Sofronis You just pointed out that if we want to be called an energy institute, we ought to address issues beyond fundamental science. We need to address issues that are related to the public's perception of technology. For that, we have the advantage of being a university, which means that we can form

a team by inviting professional faculty from other fields, such as the social sciences, to discuss how physical science can interact with social science to engage the public and encourage discussion and exchange.

Hirose If you can do it, it would be a very unique effort, especially in Japan, to work from basic science to implementation. We are expecting a lot from your institution.

Sofronis Can you tell us a little bit about the "London Hydrogen Partnership (LHP)," with whom Toyota has worked with since the last decade?

Hirose LHP was set up in 2002 to develop a network of hydrogen fuel cell (HFC) stakeholders in the capital and help develop HFC technologies in London. They are very eager to implement hydrogen in London from a very early stage, and they have a long term vision. They built stations and

accommodated buses during the London Olympics, and now are working with taxi companies to develop black cabs powered by hydrogen. They have broad visions for the future to clean up the city-including not only emissions, but also sound, since one of the biggest advantages of FCVs is that they operate in silence. Most importantly, the partnership is working with the local government to promote hydrogen, similar to the close discussions between Fukuoka Prefecture and industry, as well as the efforts in the city of Hamburg. For these big cities, the availability of a combination of public and private transport is important, especially for the coming aged society.

Sofronis Again, it goes back to your point about the societal aspect of technology. How do you view the hydrogen aspect of renewable energy versus the other aspects? Is it something that you can assess with regard to CO₂ emissions reduction?

Hirose I think some people misunderstand that our company will provide the fuel cells, and that we are able to change energy systems. In reality, the type of energy will be chosen by society. However, we cannot follow all the requirements of individual regions, so we simplify by offering the hybrid as the best solution. Regarding renewable energy, I think we need to further analyze its influence on the economy. That being said, if I pay 100 yen at a gasoline station, most of the money either goes toward tax or oil producing countries, which is not preferable for Japan (or most countries). Renewable energy can be a solution that changes direction and distributes money inside the country. Again, renewable energy is expensive because many expensive facilities need to be built, but in the

long term, renewable energy could become cheaper than gasoline or oil.

The future of research and the young generation

Sofronis You have always been innovating at Toyota. Can you tell us about the relationship between this innovative spirit and the university environment? How should we engage in the transfer of technology to get our fundamental science research out there to the real world?

Hirose Society is progressing every day. Change is inevitable for industry. This makes engineers and scientists work very hard, and their learning never ends.

Sofronis It is true that we need to change frequently as life



progresses. We're beginning to realize this at the university level too. We try to innovate by working in teams and approaching from different angles when addressing a problem. At some point, we need to engage the social component that goes beyond the laboratory.

Hirose It's important to visualize the future. The reason we invest a lot of resources in fuel cells is because in the long term, energy and sustainability will be a big issue. Find a universal target, and aim in that direction.

Sofronis Here at this university, we have a lot of young people, young scientists, with aspirations about the future. What do you think the job market in the hydrogen economy will be like for our younger generations?

Hirose In the past, energy solutions were quite simple, but in the future, they will be

much more complex, as environmental issues and economic pressure will expand the job market. It's important to be specialized in one technology, but you also need to invest interest in other fields, since energy solutions cannot be implemented without financial or sociological knowledge. If we were to hire someone, we would of course want specialists, but also individuals with broader knowledge. We expect I²CNER to play an important role and to be a base of innovation by providing such notable human resources.



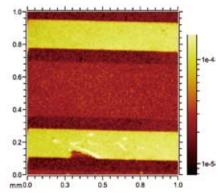
Research Highlights



Probing Active Surfaces in Solid Oxide Fuel Cells and Electrolysers by Low Energy Ion Scattering (LEIS)

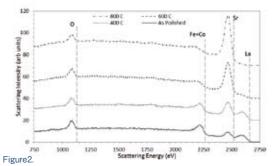
John Kilner, Tatsumi Ishihara, John Druce and Helena Tellez The Journal of Fuel Cell Technology, 13(2), pp 20 – 26, (2013)

We present examples of how our group applies Low Energy Ion Scattering (LEIS) to analyse the composition of the outer atomic layer of solid oxide electrodes, which are the very surfaces that control the exchange of oxygen between the gas phase and the device, and thus determine the performance of solid oxide electrolysers (SOECs) and fuel cells (SOFCs). We show that the surfaces of LSCF electrode materials are covered with segregated SrO after only 8 hours at 800°C. We also illustrate the first application of LEIS to a real electrochemical cell, and find evidence for La diffusion from the electrode into the electrolyte. These analyses of both bulk materials and actual cells help us understand how electrode surface composition influences the performance and degradation of SOECs and SOFCs.





Total positive ion image of micropatterned electrode half cell, showing La_{0.6}Sr_{0.4}Co_{0.2}Fe_{0.8}O_{3.4} electrodes (dark) on YSZ single crystal electrolyte (red), with Au current collectors (yellow).



Surface composition of $La_{0.6}Sr_{0.4}Co_{0.2}Fe_{0.8}O_{3.4}$ ceramics after annealing for 8 hours at different temperatures in lab air.



Experimental and Theoretical Study of Charge-Transfer Complex Hybrid Polyimide Membranes

Masamichi Nishihara, Liana Christiani, Aleksandar Staykov and Kazunari Sasaki Journal of Polymer Science, Part B: Polymer Physics DOI: 10.1002/polb.23411

Nishihara et al. have developed charge-transfer complex polymer hybrid films (CT films) as novel polymer electrolytes for high temperature polymer electrolyte fuel cells (HT-PEFCs). In this study, molecular structures of sulfonated polyimide (SPI)/dihydroxynaphthalene (DHN) derivative CT films were determined by a combined visible spectroscopy/quantum mechanical experiment. From the result of visible spectroscopy, it was confirmed that CT films, which were made of different isomeric donor molecules, have different maximum wavelengths, although the difference of the molecular structure was small. From the calculation based on the spectral result, SPI and DHNs form multiple interactions consisting of not only CT interaction, but also hydrogen bonding in multilayered structures. This insight could serve as a guide to develop a cross-linked film with high durability at high temperature.

Figure1. CT films made of different isomeric donor molecules (2,6-DHN and 1,5-DHN) and their maximum wavelength.



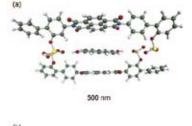


Figure2.

Molecular structures of CT films made of (a) 2,6-DHN and SPI and (b) 1,5-DHN and SPI.

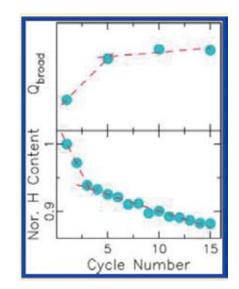
510 nm

Research Highlights

Origin of Degradation in the Reversible Hydrogen Storage Capacity of $V_{1-x}Tix$ Alloys from the Atomic Pair Distribution Function Analysis

Hyunjeong Kim, Kouji Sakaki, Hiroshi Ogawa, Yumiko Nakamura, Jin Nakamura, Etsuo Akiba, Akihiko Machida, Tetsu Watanuki and Thomas Proffen The Journal of Physical Chemistry C 2013, 117, 26543–26550 DOI: 10.1021/jp408766r

Reduction in reversible hydrogen storage capacity with increasing hydrogenation and dehydrogenation cycle number is observed in numerous hydrogen storage materials, but the mechanism behind this unfavorable change has not been elucidated yet. In this study, we have investigated the origin of degradation in the reversible hydrogen storage capacity of V1-xTi x alloys by examining local structural changes in $V_{1-x}Ti_{x}H_{2}$, x = 0.2 and 0.5, as well as pure vanadium (V) during early hydrogen cycling (less than 15 cycles). Our experimental X-ray pair distribution functions (PDFs) of $V_{1-x}TixH_2$, x=0.2 and 0.5, show significant r-dependent peak broadening, and this effect becomes stronger with each cycle number. The PDF analysis and Molecular Dynamics (MD) simulation results indicate that dislocations are responsible for such broadening of the PDF peaks, and the number of dislocations increases with cycle number. We found a correlation between a reduction in the reversible hydrogen storage capacity of V0.8Ti0.2 and an increase in the density of dislocation defects. Our PDF analysis results strongly suggest that dislocations play an important role in reduction in the reversible hydrogen storage capacity of V-based bcc alloys during early hydrogen cycling. This study contributes to elucidating the cause of degradation in the hydrogen storage capacity and improving the cyclic stability of V-Ti based BCC alloys, which are one of the most attractive materials for hydrogen tanks in fuel cell vehicles.





A Model for the Water-Oxidation and Recovery Systems of the Oxygen-Evolving Complex

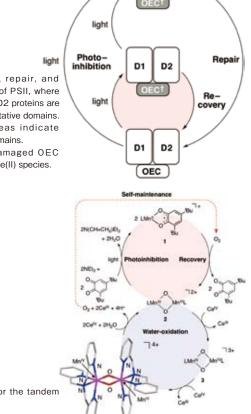
Takeshi Yatabe, Mitsuhiro Kikkawa, Takahiro Matsumoto, Hidetaka Nakai, Kenji Kaneko and Seiji Ogo Dalton Transactions (Dalton Trans.), 2014, 43, 3063/ DOI: 10.1039/c3dt52846d

In this paper, we have proposed a model for the water-oxidation and recovery systems of OEC (oxygen-evolving complex) of PSII (photosystem II) enzyme shown in Figure 1. The whole system consists of two catalytic cycles, conducted as a tandem reaction shown in Figure 2: (1) a water-oxidation cycle uses cerium (IV) ammonium nitrate as an electron acceptor to activate a dimanganese complex, with tris(2-pyridylmethyl)amine as a supporting ligand, for water-oxidation and thereby release dioxygen and (2) a recovery cycle begins with photoinhibition of the dimanganese complex but then uses dioxygen to reactivate the manganese center. Here, we have presented the recovery of the dissociated and reduced manganese complex by incorporation of atoms from dioxygen. Since the water-oxidation cycle releases dioxygen, we propose that some of this dioxygen may be utilized to recover the photo-damaged OEC.

Figure1

Photoinhibition, repair, and recovery systems of PSII, where OEC and D1 and D2 proteins are shown as representative domains. Gray-shaded areas indicate photo-damaged domains. †: The photo-damaged OEC contains manganese(II) species.

Figure2. Proposed cycle for the tandem reaction.



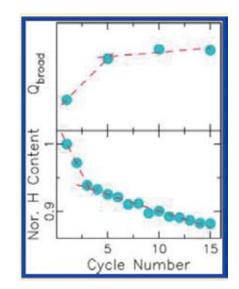
D2

Research Highlights

Origin of Degradation in the Reversible Hydrogen Storage Capacity of $V_{1-x}Tix$ Alloys from the Atomic Pair Distribution Function Analysis

Hyunjeong Kim, Kouji Sakaki, Hiroshi Ogawa, Yumiko Nakamura, Jin Nakamura, Etsuo Akiba, Akihiko Machida, Tetsu Watanuki and Thomas Proffen The Journal of Physical Chemistry C 2013, 117, 26543–26550 DOI: 10.1021/jp408766r

Reduction in reversible hydrogen storage capacity with increasing hydrogenation and dehydrogenation cycle number is observed in numerous hydrogen storage materials, but the mechanism behind this unfavorable change has not been elucidated yet. In this study, we have investigated the origin of degradation in the reversible hydrogen storage capacity of V1-xTi x alloys by examining local structural changes in $V_{1-x}Ti_{x}H_{2}$, x = 0.2 and 0.5, as well as pure vanadium (V) during early hydrogen cycling (less than 15 cycles). Our experimental X-ray pair distribution functions (PDFs) of $V_{1-x}TixH_2$, x=0.2 and 0.5, show significant r-dependent peak broadening, and this effect becomes stronger with each cycle number. The PDF analysis and Molecular Dynamics (MD) simulation results indicate that dislocations are responsible for such broadening of the PDF peaks, and the number of dislocations increases with cycle number. We found a correlation between a reduction in the reversible hydrogen storage capacity of V0.8Ti0.2 and an increase in the density of dislocation defects. Our PDF analysis results strongly suggest that dislocations play an important role in reduction in the reversible hydrogen storage capacity of V-based bcc alloys during early hydrogen cycling. This study contributes to elucidating the cause of degradation in the hydrogen storage capacity and improving the cyclic stability of V-Ti based BCC alloys, which are one of the most attractive materials for hydrogen tanks in fuel cell vehicles.





A Model for the Water-Oxidation and Recovery Systems of the Oxygen-Evolving Complex

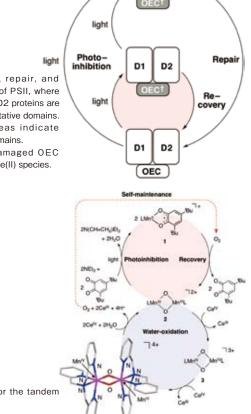
Takeshi Yatabe, Mitsuhiro Kikkawa, Takahiro Matsumoto, Hidetaka Nakai, Kenji Kaneko and Seiji Ogo Dalton Transactions (Dalton Trans.), 2014, 43, 3063/ DOI: 10.1039/c3dt52846d

In this paper, we have proposed a model for the water-oxidation and recovery systems of OEC (oxygen-evolving complex) of PSII (photosystem II) enzyme shown in Figure 1. The whole system consists of two catalytic cycles, conducted as a tandem reaction shown in Figure 2: (1) a water-oxidation cycle uses cerium (IV) ammonium nitrate as an electron acceptor to activate a dimanganese complex, with tris(2-pyridylmethyl)amine as a supporting ligand, for water-oxidation and thereby release dioxygen and (2) a recovery cycle begins with photoinhibition of the dimanganese complex but then uses dioxygen to reactivate the manganese center. Here, we have presented the recovery of the dissociated and reduced manganese complex by incorporation of atoms from dioxygen. Since the water-oxidation cycle releases dioxygen, we propose that some of this dioxygen may be utilized to recover the photo-damaged OEC.

Figure1

Photoinhibition, repair, and recovery systems of PSII, where OEC and D1 and D2 proteins are shown as representative domains. Gray-shaded areas indicate photo-damaged domains. †: The photo-damaged OEC contains manganese(II) species.

Figure2. Proposed cycle for the tandem reaction.



D2

¹I²CNER Event Reports



The Ministry of Education, Culture, Sports, Science and Technology in Japan (MEXT) and the World Premier International Research Center Initiative (WPI) Institutes, including the International Institute for Carbon-Neutral Energy Research (I²CNER), represented WPI at the 2014 American Association for the Advancement of Science (AAAS) Annual Meeting held in Chicago, USA February 13-17. AAAS is the world's largest general scientific society and is the publisher of the journal "Science." The theme for this year's meeting, which was the 180th AAAS Annual Meeting, was "Meeting Global Challenges: Discovery and Innovation." The WPI Institutes and MEXT hosted the WPI booth as part of the Japan pavilion, which was organized by the Japan Science and Technology Agency (JST). Over the course of the three-day exhibition, a wide range of participants,



including scientists, administrators, and lawmakers, visited the Japan pavilion. On February 14, WPI and RIKEN held a workshop with the theme, "Build a Career in Japan!" In the workshop, Mr. Hideki Iwabuchi, Director, WPI / Office for Promotion of Basic Research, Research Promotion Bureau, MEXT, outlined the WPI program and described exciting career opportunities in Japan for foreign researchers.



I²CNER & ACT-C Joint Symposium ~Advanced Molecular Transformations for Sustainable Energy Future~ Ito Campus, Kyushu University



On January 30, 2014, the International Institute for Carbon-Neutral Energy Research (I²CNER) co-organized the "I²CNER & ACT-C Joint Symposium" with the Advanced Catalytic Transformation program for Carbon utilization (ACT-C) of the Japan Science and Technology Agency (JST). The symposium was held in I²CNER Hall on the Ito Campus of Kyushu University and was attended by 177 people, including many international guests. After opening remarks by the Executive Vice President of Kyushu University, Prof. Yukio Fujiki, I²CNER Director Prof. Petros Sofronis and ACT-C Director-General Prof. Toyoki Kunitake introduced the latest research activities of I²CNER and ACT-C, respectively. The plenary lectures were given by Prof. Ei-ichi Negishi of Purdue University, 2010 Nobel Prize





Laureate in Chemistry, and Prof. Benny D. Freeman of the University of Texas at Austin. In the afternoon session, various researchers of I²CNER and ACT-C gave presentations on their latest research f in d in g s. The symposium concluded with a poster session in which participants actively exchanged ideas concerning their research activities.