ETH

Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Genehmigung des Forschungsplans

(Definitive Zulassung zum Doktorat)

Approval of the Research Plan

(Full admission to doctoral studies)

Studierenden-Nummer *student number*	16 -	950 -	073
Name *family name*	Xu		
Vorname *first name*	Hong		
Departement *department*	D - CHAB		

Der Forschungsplan wurde eingesehen und angenommen durch:
The research plan has been seen and approved by:

Prof. Thomas J. Schmidt	13.2.18	
Name Dissertationsleiter/in *Name of supervisor*	Datum *Date*	Unterschrift *Signature*

Name Bevollmächtigter Doktoratsausschuss *Name of representative of doctoral board*	Datum *Date*	Unterschrift *Signature*

Für Kandidaten mit weiteren Zulassungsbedingungen:
Die Zulassungsbedingungen müssen **vor** Genehmigung des Forschungsplans erfüllt sein!

For candidates who have to fulfil further conditions of admission:
These conditions must be fulfilled ***before*** *the research plan can be approved!*

Frist für Einreichung des Forschungsplans

Frühestens nach erfüllen und offiziell verfügtem Bestehen der Zusatzbedingungen, spätestens ein Jahr nach der Einschreibung

Vorgehen zur Genehmigung des Forschungsplans

Lassen Sie dieses Formular und den Forschungsplan von Ihrer Leiterin / Ihrem Leiter unterzeichnen und senden Sie danach beides an das zuständige **Studiensekretariat**. Dieses kümmert sich um die Unterschrift des Bevollmächtigten des Doktoratsausschusses und schickt das Formular anschliessend an die Doktoratsadministration.

Deadline for submission of the research plan

Only after having passed and received official notification of having successfully fulfilled the further conditions of admission, one year after registration at the latest.

Procedure for approval of your research plan

Please ask your supervisor to sign this form and your research plan and send both to the **Study Administration Office of your department**. They will take care of having it signed by the representative of the doctoral board and will forward it to the Doctoral Administration Office afterwards.

PAUL SCHERRER INSTITUT

Subsecond dynamics of liquid water transport in polymer electrolyte fuel cells revealed by 4D X-ray tomographic microscopy

SNF Project No.166064

Research plan for the PhD dissertation of

Hong Xu

20th Feb 2018

		Date & Signature
Advisor:	Prof. Dr. Thomas J. Schmidt	14.2.18
Co-advisors:	Dr. Jens Eller	14.02.2018
	Dr. Felix Büchi	14.2.18 F. B
PhD candidate:	Hong Xu	Hong Xu 14/02/2018

Motivation

Polymer electrolyte fuel cells (PEFCs) have been recognized as efficient energy converters which turn the chemical energy stored in hydrogen fuel into electrical energy with low emissions, operating temperatures and ambient noise [1]. Thus PEFCs are a key element for a future, secure, and sustainable clean energy economy [2]. While fuel cells are becoming competitive in emerging markets, commercialization can be expanded with improvements in terms of durability, performance, and cost reduction [3].

A PEFC is typically a sandwich of two flow field plates with flow channels that are separated by a membrane electrode assembly (MEA). The MEA consists of an ion-conductive membrane, two gas diffusion electrodes with dispersed catalyst, and two gas diffusion layers (GDLs) on both sides of the electrodes [4]. The GDL is porous to supply reactants to the electrodes and drain the water generated during operation, which can saturate the pores of GDL and hence impede the gas transport to the catalyst. From the perspective of cell performance improvement, the water management in the gas diffusion layers is therefore vital to ensure sufficiently low reactant gas transport resistance in the GDLs in order to achieve the high current density operation that is necessary for high power automotive applications [5].

X-ray tomographic microscopy (XTM) has been employed to image the water distribution during cell operation and its capabilities have successfully been demonstrated for water management investigations due to its high spatial (few micrometers) and temporal resolution (several seconds) [6]. In order to study the water transport mode and water dynamics in GDL during transient operation, sub-second *operando* 4D imaging of realistic cells needs to be developed.

Objective

The aim of this dissertation is the development of *operando* subsecond XTM methods in order to reveal the water transport modes and dynamics of liquid water in the GDL during transient operation of PEFCs.

The first step is the understanding of dominating water transport modes in GDL. It remains still unclear if the produced water is transported dominantly by capillary pressure or by a root-like merging of condensation clusters [7, 8]. For this application tomographic scans in the order of $1 \sim 2$ s are required for imaging the water clusters in the GDL and clarifying the driving process. Secondly, the water dynamics in the GDL during transient operation need to be further explored. For imaging the response of the water distribution as function of the change in operation conditions, time series tomographic scans of about 0.5 s are required. Thirdly, since the liquid water distribution fluctuates in time, the rate of oxygen transport to the cathode catalyst layer also fluctuates, which results in unstable power density and/or efficiency [9]. This phenomenon will be studied by coupling fast *operando* XTM imaging with electrochemical measurements including power spectra. The liquid instabilities will be correlated with the power spectra of time series data with a temporal resolution of 0.1 s.

In order to study the scientific questions proposed above using very fast XTM scans (down to ~ 0.1 s scan time), the *operando* X-ray imaging setup is further developed in collaboration with the TOMCAT beamline (X02DA) of the Swiss Light Source (SLS). The current imaging setup at TOMCAT provides tomographic scans with reasonable image quality and 1 ~ 2 s temporal resolution under monochromatic beam mode. The beamline supports fast scans with temporal resolution down to 0.05 s, limited by the present hardware of the rotation stage. But at such low scan times, the image quality is presently not adequate for post processing. Thus a low contrast-to-noise (CNR) image processing workflow has to be developed, which requires the identification of image filters and the analysis of feature detectability for liquid water [10]. A new high numerical aperture microscope is planned to be installed at TOMCAT beamline and expected to improve the image acquisition for XTM in terms of better image quality and faster acquisition time.

Research schedule

The project is divided into four main topics. The first part of the thesis is dedicated to develop a low CNR segmentation workflow with water feature detectability analysis and imaging condition optimization, which mostly has been done within the first year with two SLS-proposal based beamtimes (20170501, 20170918) and preliminary results have already been published [10].

In the second part of the project I aim to understand the dominating water transport mode in GDL with scanning times of 1.6 s. The present *operando* imaging setup will be exploited for the scheduled SLS beamtime (20180614-20180615).

The third part of the project is to study how the water saturation transforms under transient operation conditions. Here faster tomographic scans of 0.5 s are required and the SLS beamtime is expected in the fourth quarter of 2018.

Based on the accumulated knowledge of the second and third part, the fourth part of the project will be about further expanding the understanding of the power fluctuation and its correlation to liquid instabilities of operating PEFCs. Even higher temporal resolution of 0.1 s is required and the SLS beamtime will be scheduled for the second quarter of 2019.

Time frame

Task	2017 (1st year)				2018 (2nd year)				2019 (3rd year)			
	01-03	04-06	07-09	10-12	01-03	04-06	07-09	10-12	01-03	04-06	07-09	10-12
1.1 literature review												
1.2 introduction to electrochemistry lab techniques												
2.1 practice of present PEFC test bench												
2.2 learning of TOMCAT beamline operation skills												
3.1 XTM Imaging condition optimization		#			*							
3.2 development of low CNR segmentation workflow												
3.3 water feature detectability analysis			#									
4.1 dominating water transport mode analysis in GDLs						*						
4.2 water dynamics investigation under transient operation								*				
5.1 power fluctuations and liquid phase instabilities study										*		
6. writing of PhD thesis												

#operated SLS beamtime
*scheduled or planned SLS beamtime

Notes: officially started work at PSI on 1st Dec 2016 and matriculated at ETH Zurich as PhD student on 20th Feb 2017.
Gray scale represents for the intensity of corresponding work load.

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