Applicant Research Update Summary

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March 14, 2014

Contents:

1. Research Interest

I am interested in microscale transport research, including heat, mass transport and fluid dynamics since I found transport is so philosophical to explain a lot of phenomena. I want to be a micro/nano innovator, so I think transport would be a good point to start.

2. Research Update Summary

For the past four months, I tried to improve my understanding in micro scale transport. Above topics are usually studied by thermal physicist. Point 1, 2 is my reading content in last semester. Point 3, 4 is for senior design preparation.

1. Interface science
   Interface science is the key to understand fluid-solid transport. We not only can study the key questions that concerning the bubble growth and separation on nano structures, but also can study the microchannel fluid better. It pushes the fluid transport research into micro scale.

2. Micro scale solid thermal transport
   Learn about the basic concepts, including carrier statistics (Boltzmann and ensembles) through the MOOC offered by Prof Tim Fisher on Nanohub.org. Then I could understand the findings of different papers.

3. Nano structures and basic fabrication
   Nano structure put the material several unique transport properties. So learning about the structure and fabrication is the first thing to do. I literature reviewed all the carbon-silicon anode nanostructures.

4. Multi-scale modeling for thermal transport.
   After I read about the electrode structure, I found there is no clear investigation on the micro-meso scale modeling for the real electrode. The multi-scale research is in vacancy because it requires expertise in both nano materials and transport modeling. I pick this as my degree paper because it enhance my understanding of both.

   Below is my schedule and progress table.

Time	**Action**	**Content**	**Goal**	**Progress**
Oct-Nov	Seminar & Reading	Interface Science(Including Chapters of *Intermolecular and Surface Force*)	Understand solid-fluid interface	Fulfilled the seminar and got invited for summer intern in Alberta. Finished four chapters of Book.
	Course	Fundamental to Fuel Cell	Understand electrochemistry	Fulfilled.
Dec	Personal	Application to Graduate Schools	Get the research position fits me most.	Fulfilled.
	Course	Thermal Energy at Nanoscale-by Prof. Tim Fisher(Online MOOC)	Understand the fundamental to microscale transport	Finished three chapters and will keep on when get back Tsinghua.
Jan	Reading	Statistical Mechanics, Quantum Mechanics	Facilitate above course	Waiting for taking courses back in Tsinghua.
	Research	Literature Review for Lithium-ion Battery Nanoscale Electrodes and Transport	Prepare for Senior Design Project	Working on thesis proposal.
Feb	Contest & preparation	Linear Optimization and Network Analysis,ICM (Interdisciplinary Contest in Modeling) held by US COMAP	Apply mathematics to modeling complex system	Accomplished a report. The rating is undergo.
	Research	Engineering Design Perspective for Li-B Battery Electrode	Applying Design Science and Modeling for Nano science	Worked out the framework, picked mathematic method, and plan to do it later after senior design
Mar	Research	Multi-scale modeling for nanostructured electrode thermal transport	Learn about cross-scale modeling (HMM, Network, RMG, etc)	Literature review(defined as degree paper thesis)

All my research updates that I emailed to the faculty that I am interested in.
Online version: http://www.letianwang.me/1/category/recent-updates/1.html

Update No.1- Dec 25th

In the long term I would love to understand the microscale transport. Thermal physicist works on solid and fluid two types of transport.

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1. For solid part, I am aware of my lack in higher-level physics. Therefore, my first priority work would be knowledge replenishment.
    a. I joined the online course of Thermal Energy at the Nanoscale provided by Prof. Fisher in Purdue. It offered the most important concepts within short 5 weeks.
    b. I find using LAMMPS and Material Studio to simulate conduction is not hard, but a higher mastery of statistic mechanics is necessary, and I selected a course next term.
    c. **Problem A**: One of my goal is to achieve the device-level demonstration of the cooling for nanoscale hot spot with the integration of both the carbon nano materials and nanoscale fluid transport. There are emerging novel phenomena on nanoscale thermal properties. But I do not have a clear roadmap yet.

2. Fluid: For me, I had some preparation basing on my undergraduate study. Recently, my interest mainly falls on interfacial phenomena of nanostrucutures. I had read about the papers on following topics and had some problems:
    a. Intermolecular forces, which is about the contact angle properties, comes into heat transfer researcher's view recently due to the emergency of hydrophobic surfaces. I read about the adhesion force of nanostructured surface and droplets with different properties by group in Alberta. It might offer insights on droplet and superhydrophobic surface separation.
    b. Prof. Ronggui Yang's recent discoveries indicated the fluid transport is also important in addition to the intermolecular forces for phase changes. He found only the combination study of fluid replenish and intermolecular forces could account for the influence of nanostructure on phase change. He is trying to study droplet spreading on nanostructured surfaces to combine both of two factors. His preliminary work indicates that there are monotonic relationship between the spreading spead and heat flux.
    c. A design approach for sustaining vapor phase for a immersed superhydrophobic surface has been reported by Prof. Patankar in Northwestern. This work brings the contact angle research into the more realistic heat transfer application.
    d. CNT has hydrophobic properties that transport liquid through its body without frictions, which is studied some time ago by Berkeley.

Researchers has demonstrated the application on water purification and medical injector now.

e. **Problem A**: The importance of active wetting in cooling system. I am not aware of where could the necessity of active on-spot cooling will beat the extra cost it brings.
f. **Problem B:** The cooling challenge of wearable and flexible electronics devices. The fluid transport as well as interface material are two challenges in my view.

3. After the discussion of my mentor, my senior project is determined as Silicon-CNT hybrid anodes for Lithium-ion Batteries. It mainly originates from our group's transition to nano scale transport and energy conversion. I expect research training on nano fabrication as well as ion diffusion and system analysis.

Update No. 2-Jan 6th

A basic physics concepts and principles in nanoscale solid transport.
B my senior design topic choice

A. physics on nanoscale thermal transport.

Content:

1. The online course Thermal Energy at the Nanoscale offered by Prof. Tim Fisher. I am half way in Week 2 lectures.
    a. Lecture 1: Lattice Structure, Phonons, and Electron
        i. Lattice vibration and phonon (acoustic and optical phonon, intro)
        ii. Free electron and band theorem (intro)
    b. Lecture 2: Carrier Statistics
        i. Phonon and electron density of states (intro)

2. Statistical physics (Thermodynamics and statistical mehcanics by Wlater Greiner Springer; Introduction to Statistical Physics, Kerson Huang, 2ed)
    a. Phase space and entropy
    b. Fermi, Bose and Boltzmann system and distribution (classical description, most probable distribution aspect)
    c. Ensemble: phase space density and Liouville theorem, the difference of different ensembles.

3. Solid state physics (Chinese-Kun Huang, English-Charles Kittel)
    a. Lattice geometry and reciprocal lattice
    b. Atomic binding and Crystal

Comments:

1. I found the introduction given by Prof. Fisher is highly condensed. Therefore I have to dilute it by reading several other books. Originally, I planned to took them next term, but now, I need to learn by myself. Mult-dimensional vacancy on physics is hard, however, since I have such experience working on two projects, I believe it would work out better later.
2. Apparently, I am still at the entry of the nanoscale thermal transport, where I need to use the combination of quantum mechanics and classical mechanics to understand the transition. I found it interesting to study the evolution of people scientific understanding towards a specific topic. Boltzmann is great but he also has failed hypothesis like ergodic hypothesis.

B. Senior design on lithium-ion battery nanostructures:

I reviewed the cathode and anode research progress . In order to be coherent with our lab's work in solar cell, my current focus is on Si-C anodes. The silicon has good lithiation storage ten times of current graphite anode capacity, however it suffers from pulverization caused by its 400% volume change. Carbon material has excellent mechanical flexibility that could support silicon. Also carbon served electron transport pathway to improve the conductivity. Now I am researching on basic fabrication process of current Si-C structure. A more detailed presentation is in preparation.

There are two points that I would love to note.

1. It is good to find out there are research groups in Tsinghua working on silicon and carbon anodes too, which reminds me that searching for possible cooperation is really important especially in the era of interdisciplinary research. From most innovative researchers experiences, I believe communication and mutation would help to develop unforeseeable solutions to current challenges.
2. This piece of research may not be explorative or deep in theoretic. But considering my previous simulation and modeling work, basic experimental operation and first hand understanding of nanoscale materials would be beneficial to my future research. Also in a long term, it could help me to shorten the bridge of research and technology.

Update No.3-Jan 23rd

1. Si-C anodes for high capacity lithium-ion batteries: nanofabricaton and supercapacitors
2. Engineering design and electrode material
3. Transport and battery
4. My presentation(see my webpage:http://www.letianwang.me/current.html)

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1. **Understanding:** Si-C is a good starting point to have some understanding of nano fabrication as well as nano transport.
    a. Silicon has unique semiconductor properties with various applications. Also, silicon fabrication has received benefit from massive production in circuits.
    b. Carbon nano materials has great potential to be connecting, supporting and even functional application in nanoscale devices.

2. **Understanding:** I had some attention put on the supercapacitors. By reading the new released paper on CDI capacitive deionization for water desalination by Prof. Santiago in Stanford. The ion transport method could be borrowed from it.In situ spatially and temporally resolved measurements of salt concentration between charging porous electrodes for desalination by capacitive deionization

3. **Idea:** Electrode material innovation bases on design concepts
    a. An idea matrix and innovative operator method is described in paper : IDEA MATRIX AND CREATIVITY OPERATOR, Victor Tang, Jianxi Luo, ICED 2013.
    b. Silicon-carbon anode geometries follows a matrix + operator pattern.
        i. Material Matrix: Si NW, C NW, Si NP, C NP, Si Nanosheet, C Nanosheet.
        ii. Operator: Addition, subtraction, hierarchical, encapsulation
        iii. Maybe there is some interesting relation therefore we can provide design guide to nano materials.

4. **Idea:** Transport research as well as systematic research in lithium-ion is rare. Two possible topics could be done.
    a. If we use lithiumnation-delithiumnation model by material science researcher plus transport theories in thermal science, there will be theoretical explanation to the lithium-ion batteries performance.
    b. Thermal transport in nanoscale material is not well understood, which is critical for systematical modeling the battery thermal stability.

Update No.4-Jan 31st

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1) Firstly, I have been working on the MCM (The Mathematical Contest in Modeling) held by COMAP in US. Taking part in this contest, I am trying to review and further improve my mathematics at the end of my college life. In another aspect, I am challenging a new topic.

2) I noticed the newly released paper *Nanoscale thermal transport. II. 2003–2012* by several renowned researchers in thermal transport field.It is a great guidepoint for me to further walk into this field. It had reviewed the interfacial transport, the phonon

transport and nano material effects on it, and lastly the experimental advancement. The authors focused on the interfacial transport and offered me a better understanding of how this topic evolved. But unfortunately, I could not master the detailed information, so there is much more to prepare.

3) I have been keep searching detailed research topics for my senior design. I found the paper *Combined Microstructure and Heat Conduction Modeling of Heterogeneous Interfaces and Materials* by Prof. Fisher gives a good modeling connecting the microstructure and continum theories of transport, which could help me on reserching transport in electrodes. Also, I found what I have learnt in Purdue, the Effective Medium Theories has been used again in this work. Everything is so wonderful!

4) Finally, I has been at home preparing for the upcoming Spring Festival, the last one I had with my families. In China, Spring Festival is like Christmas, family members from all over the country went back home.

Update No.5 –Feb 17th

1. Lithium-ion electrode thermal modeling
2. Network Analysis

Some of the updates are related to microscale transport and some are not. But all the updates are related to my long term plan: being an innovative and entrepreneurial researcher.

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1. I discussed the transport modeling of Lithium-ion Battery with Dr. Yonghuang Ye in NUS, Singapore. He answered my questions concerning the macro mathematical model of transport in Lithium-ion battery. He thinks there are limited research linking microscale structure and transport.
2. Our team has completed Network Analysis towards 2014 ICM. It is a challenging problem since none of us had knowledge on network analysis and we need to solve the problem in 4 days in a report. But I found learning new knowledge is not that challenging and understanding the challenge is much more important. It's exciting that Prof. Jianxi Luo working on network analysis are impressed by our solutions and interested in our finding. You can find our more on my site: http://www.letianwang.me/network-analysis.html

Update No. 6-Feb 25th

Summary

Update No. 7-Mar 13th

My degree paper topic is defined as the multi-scale thermal transport modeling for nanostructured electrodes. The major work is inspired by the process of my literature review of nano material and the paper *Combined Microstructure and Heat*

Conduction Modeling of Heterogeneous Interfaces and Materials . The content is listed below:

1. Relate the micro structure to the transport properties for nano electrode. Understanding how specific nano structure like coating, core-shell, hierarchical will change the thermal transport.
2. Choose appropriate parameter transmission framework (network, HMM and others) for micro to meso and macro. Now the candidate model is multi-scale network method.
3. Using macro scale simulation (COMSOL) to analyze how the micro and mesoscopic geo parameter will affect the whole battery performance.

Research Memos-

1. **Multi-scale modeling**

   With the emerging of nano science, scientist collected a lot of interesting information from micro structures, which is currently only used in nanoscale. However, the engineering paradigm is still macro modeling. How to accommodate the new information became a critical issue. I am trying to understand the "multi-scale". I worked on material transport properties for my senior design. I am trying to link the nano structure material transport properties to macro properties. But I just started and looking forward to discover more topics to talk about.

2. **Complex system and design optimization**

   Also , I am interested in thinking about engineering from complex system and using data analysis . Complexity is one of the major characteristics for the future technology development. Using data tools to facilitate science exploration and engineering design is my prospective for the future. As a consequence, I am reading about graph theories and applied them into a complex network analysis. You may find it out on my web http://www.letianwang.me/network-analysis.html. I also came up with an idea using data to facilitate the electrode research for Lithium-ion battery: http://www.letianwang.me/engineering-design-for-nano-electrode.html

Lectures I have audited:

Jan, 2014
Lecture: Nanowire Devices for High-Performance Energy Storage
Lecturer: Liqiang Mai, Professor, WUT-Harvard Joint Nano Key Lab

Dec, 2013
Lecture 1: Multiscale Simulations and Ultrafast Characterization for Nanoscale Heat Conduction
Lecture 2: Phase-Change Heat Transfer at Micro/Nanoscale: from Fundamentals to Manufacturable Devices
Lecturer: Ronggui Yang, Associate Professor, Mechnical Engineering, University of Colorado, Boulder

Nov, 2013
Seminar: Interfacial Science and Technology in Energy Industry
Lecturer: Qingxia (Chad) Liu, Professor, Chemical and Materials Engineering, University of Alberta

Oct, 2013
Lecture: Simulation of thermal and thermoelectric properties of carbon nanomaterials
Lecturer: S.Watanabe, Department of Material Engineering, The University of Tokyo