

# Report on Long-term Overseas Dispatch

Department of Materials Engineering, 2<sup>nd</sup> grade of Ph.D.

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## Abstract

I have conducted the long-term overseas dispatch at the group of Professor Anna C. Balazs in University of Pittsburgh, PA, USA. I report the background, research, life in Pittsburgh in this document.

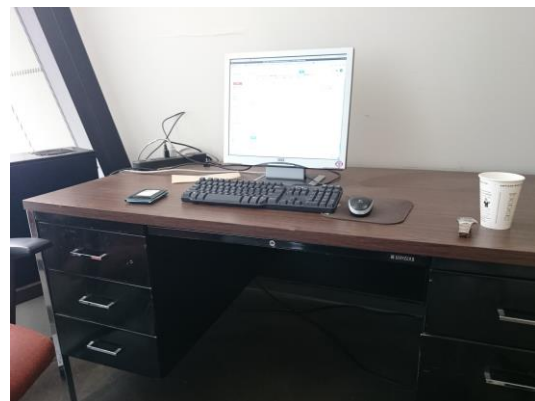
## Background

The research group lead by Prof. Balazs majors in computer simulation of soft matters including gels. On the other hand, Yoshida-Akimoto group, which I belong to, majors in self-oscillating gel, which shows autonomous periodic volume change driven by oscillatory chemical reaction. These two groups have done several collaborating research, in which some oscillatory behaviors of gel were simulated by gel lattice spring model (gLSM) specially modified for stimuli-responsive gel.

This time, my supervisor sent an e-mail to Prof. Balazs, and she kindly accepted my dispatch.

## Research

It was first time for me to do computational research, so she introduced to me a software called LAMMPS, which is relatively easy for amateurs to manipulate, and I started dissipative particle dynamics (DPD) simulation using this software. In the first 2-3 weeks, a postdoc gave me a completed script for simulation of binary phase separation, and learned the LAMMPS commands. In parallel, I also studied C++, which is necessary for enhancement of LAMMPS and creation of data file of initial “beads” positions.



Working space

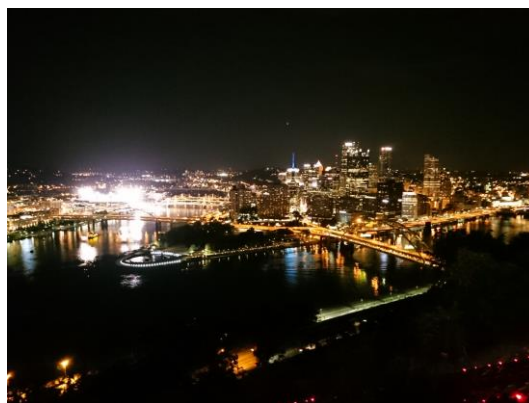
After that, I worked on writing LAMMPS script according to a published paper which mentions the DPD simulation of gels' volume phase transition behavior. This task was a repeat of trial and error and needed much endurance. As a result, it took about 2 weeks to find only one easy mistake in

the script, and only 1 month remained after finishing this task.

During the remaining term, I tried to reproduce the gels' shrinking pattern formation, which is confirmed under the condition that dispersion of solvent molecule is restricted by a formation of dense skin layer in the surface region of gels. Especially, the reproduction of skin layer was very challenging. It must be dense enough to restrict the solvent molecule dispersion, and soft enough to change its shape, and the tuning of the parameters of beads to realize this condition was difficult. Finally, I tried mainly two methods, and they worked well to a certain level.

## Life in Pittsburgh

Pittsburgh is a city nestled between two rivers, and called “city of steel” as Pittsburgh boasted a steel industry in the past. The Oakland district, where University of Pittsburgh exists, is a safe town for students, having several universities including Carnegie Mellon University. I stayed in a dormitory, which stands in the campus of university, and many foreign students also were staying there. There were many restaurants around the dormitory, and I had lunch and supper mainly in these restaurants. Additionally, students can use most of public transportations and institutions for free or with some discounts, so the city is very comfortable for every student.



Night view of Pittsburgh

In Pittsburgh, Japanese have close communication, and we can get much important information for daily lives from the website “Pittsburgh Benri-chou” (ピッツバーグ便利帳). They hold BBQ party once or twice a month, it was a trigger for start enjoying the life there.

On weekdays, I went to the office at 10 am and leave at 7 – 8 pm. At first, I could not get used to the research style without any chemical reagents, and often thought about the research at my group when the simulation resulted in many errors. Balazs group has group meeting once a week, and all member present their research progress. Most of the members were dealing with writing paper, and the activeness of discussion and the high speed of research and its cycle were surprising.

## Acknowledgement

I appreciate Dr. Balazs and Dr. Yashin kindly accepting my long-term dispatch, and the post-doc students teaching me how-to of computational research while they are busy with their own research. And I also specially thank teachers in MERIT program, Dr. Yoshida and Dr. Akimoto for giving me a great opportunity.