（別紙様式２）

フォトンサイエンス国際卓越大学院プログラム（XPS）

光科学特別実習　報告書

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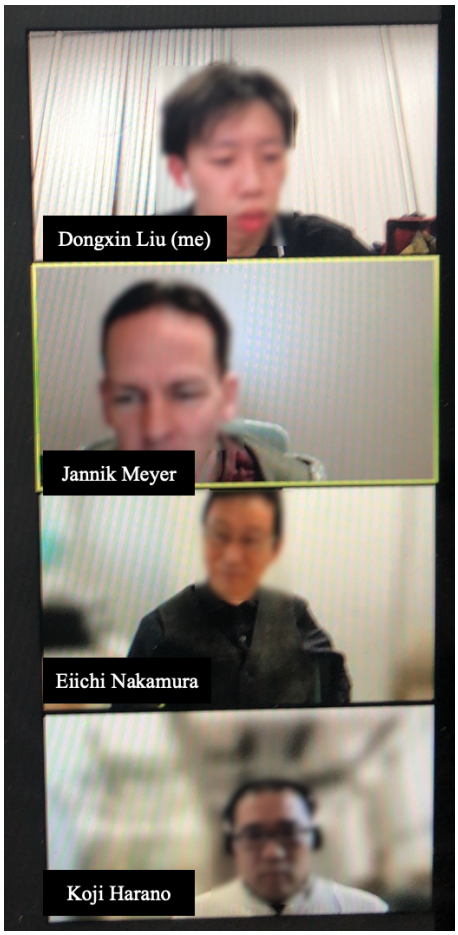

As a Special Training in Photon Science, I attended Pacifichem2021 via Zoom and presented a poster titled “Experimental elucidation of non-thermal melting in electron crystallography of organic microcrystals” as a part of the session “Direct Visualization of Chemical and Self-Assembly Processes with High-resolution Microscopy.” The conference is held every four years for attendees from all over the world from all the fields of chemistry, and Pacifichem2021 was postponed from last year due to the pandemic. The conference was planned to be held as a hybrid style via both on-site and Zoom but eventually the conference committee decided to hold this time exclusively via Zoom. This decision was partially sad, losing opportunities to meet people face to face but at the same time allowed easy attendance from anywhere on the earth, which I believe contributed a lot toward the success of “electron microscopy (EM) division” of Pacifichem2021. Although this division is still growing and relatively small, it could gather people as much as thirty or forty, being as active as other popular sessions.

What I presented was about the interaction between electron beam (e-beam) and materials, especially the initial process induced by e-beam during a small amount of e-beam irradiation and the elucidation of the mechanism of the physical or chemical phenomena taking place. My research topic focuses on interdisciplinary fields of chemistry and EM so an opportunity to discuss the results in depth has been rare and this conference has been an invaluable chance, bringing electron microscopists, physicists and chemists together at a time.

While e-beam has been utilized as a probe to reveal structures or dynamics of molecules at atomic resolution, for example, in cryo-EM, electron diffraction (ED) or transmission EM, such methods typically suffer from loss of information. At the late stage of e-beam irradiation, information loss is ascribed to irradiation damage induced by e-beam according to the type of specimens but the effects of damage are unavoidable even within the initial process of e-beam irradiation. During the initial process, motion of individual molecules caused by e-beam limits the resolution and recent efforts with the focus on the movement of EM grid or the ice layer achieved a breakthrough of high-resolution in the field of cryo-EM. However, the physical or chemical mechanism behind the motion of EM grids, ice layers or even target molecules themselves in electron microscopy is still elusive. In this work, I showed the dynamics of each molecule during the initial process induced by e-beam can collectively be understood as a non-thermal melting. For the investigation of the initial process, I conducted kinetic analysis of e-beam-induced fading of ED patterns, which is one of the most structure-sensitive methods to capture changes in specimen and studied a wide variety of organic molecules and inorganic matters. I found the corresponding activation energies are small for a thermal process regardless of the compounds, indicating the fading of ED patterns is a non-equilibrium process induced by e-beam irradiation. I further found a statistically significant correlation between the frequencies of the fading of ED patterns and the melting entropies of bulk crystals, suggesting the motion of individual molecules

during the initial process can macroscopically be recognized as melting. Beyond the statistical analysis, a physical relationship between the frequencies and melting entropy could be established to confirm the proposed non-thermal melting and activation energy was shown to be related to melting enthalpy and melting temperature by analysis using machine learning. Those results could provide a practical strategy in achieving further improvement of EM and ED in terms of resolution, and a fundamental principle in discussing the interaction between e-beam and both organic and inorganic compounds.

As shown in the top photo, luckily, one of the experts of this fields from physics side, Prof. Jannik Meyer, came by my poster and I could present the results to him along side of my mentors, Prof. Eiichi Nakamura and Prof. Koji Harano. From the discussion, I could gain the insight about how the obtained results should be presented as a paper so people from various fields would understand the content and benefit from the findings. In addition to him, I also had an opportunity to discuss with Prof. Dominik Lungerich, who was working in the University of Tokyo as a postdoctoral fellow in the same lab with me and currently in Yonsei University as a Professor. As a former-insider, Dominik pointed out several critical points, which I'm currently working on to improve the content of the paper for the results. Besides the poster and talk sessions, I could have opportunities to join personally arranged discussion with Prof. Jannik Meyer and Prof. Haimei Zheng, thanks to Prof. Eiichi Nakamura. During the sessions, discussion related to both the content of the poster and another topic, which is currently available as a preprint (https://arxiv.org/abs/2110.02530), was done and led to further improvement of the preprint and the ideas were summarized in new versions of the preprint.

To summarize this experience, I believe this is the best conference I have ever attended. Although majority of the conference was from chemistry, thanks to my mentors, the "cinematic chemistry" sessions gathered important scientists of the interdisciplinary field and I could attend their lecture at once from my laptop. No other conferences have provided such a fulfilling time and it was really a nice opportunity to join the session.