Internship Report

Department ：Graduate School of Frontier Sciences, Advanced Materials Sciences
Terashima ・ Ito lab.
Year, Student number, Name ： D3, 47-217003, Yuki Inada
Supervisor ： Kazuo Terashima
Mail ： inada-yuki021@g.ecc.u-tokyo.ac.jp
Phone number ： 04-7136-3797

1．Outline of Internship

Institution ： Zeon Corporation, R&D Center
Term ：2023/02/01〜2023/03/31
Form ： Hybrid (online and in-office). Two days a week in-office at Zeon Corporation R&D Center.
Person in charge ： Mr. Tetsuaki Matsubara / Mr. Yasuo Tsunogae
Supervisor ： Dr. Yuki Ono / Mr. Riku Shirota
Themes ：
(1) Acceleration of rubber compounding search program
(2) Estimation of three-dimensional pigment distribution based on SEM images of toner cross sections
Reason for application ：

　ZEON Corporation mainly handles polymer materials such as synthetic rubber and resin materials. My university research theme is materials informatics for inorganic materials, and I thought that my experience in research on data analysis of organic materials, a neighboring field of inorganic materials, would broaden my perspective in my future research activities. I also hoped to participate in this internship because I expected to gain practical experience by working on data analysis that assumes actual use in companies.

2．Themes and Results

(1) Acceleration of rubber compounding search program

　ZEON Corporation is attempting to use machine learning to quickly propose rubber compounding that meet the requirements of desired physical properties. Using machine learning models that predict physical properties from rubber compounding, Mr. Shirota, who was supervisor during this internship, created a program to propose rubber compounding with desired physical properties. This program was created with the goal of displaying the prediction results in real time, but it had a problem with insufficient execution speed, taking about one minute.

　As an internship theme, I modified the program to allow more flexible adjustment of the number of candidates to be searched. In addition, I proposed and implemented the hill-climbing algorithm, a searching algorithm that performs better when the search space is larger. As a result, the program was able to output about 100 predictions in a few seconds, which is a practical execution speed.

(2) Estimation of three-dimensional pigment distribution based on SEM images of toner

cross sections

 The state of the toner's charge is important in the production of high-quality toner. In the manufacturing process of toner, there are cases where variations or reductions in the state of charge occur. There is a need to observe and analyze the internal state of the toner to investigate the cause of these variations or reductions. However, the data obtained on the inside of toner are cross-sectional SEM images, and it is difficult to directly obtain three-dimensional information.

 In this study, we attempted to infer three-dimensional information about toners from the radius of the cross section, and the position and size of pigments obtained from the cross section of the toner. We modeled a spherical toner and its internal pigment distribution, performed simulations under various conditions, and compared the results with data from the actual toner. The relationship between the size of the toner and the radius of the cross section, the bias in the arrangement of pigments inside the toner, and the volume occupied by pigments inside the toner were analyzed.

 As a result, it was possible to estimate the size of the original toner from the radius of the cross-section, to determine whether the pigments are uniformly distributed within the toner, and to estimate the percentage of the volume of pigments in the toner from the percentage of the area of pigments in the cross-section. Some elements have not yet been incorporated into the modeling, and it is expected that more accurate understanding of the toner's internal information will become possible by developing the simulation to be more in line with actual conditions.
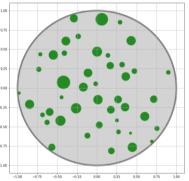

Figure. An example of toner cross section generated by simulation. Green dots represent pigment.

 The results were presented in a final internship debriefing session.

3. Comment for internship

 During this internship, I was able to experience firsthand how the use of data in corporate R&D is steadily advancing, and I feel that it was a very good stimulus. At the same time, I recognized that there are issues that are difficult to be solved immediately, such as data accumulation and maintenance, and realized the need for future development in both data collection and analysis.

 During the course of the internship, the opinions of experts in various fields greatly helped me to decide how to proceed with the analysis and what kind of program would be useful. In the theme of the rubber compounding exploration program, we were able to deepen our understanding of the data by observing how rubber is actually made and how the data is collected. In addition, I was able to participate in discussions on the theme of SEM image analysis, where the policy on how to analyze had not yet been decided. This experience made me realize the importance of exchanging opinions from various viewpoints. I realized how important it is to actively try to understand topics in fields outside of one's own expertise and, conversely, to explain methods and results in an easy-to-understand manner to people with different fields, in order to have fruitful discussions.

 The above points are important in daily research, and I was able to reaffirm their importance

more clearly this time by participating in a research project involving many people in a different field from my usual one. I believe that this internship provided me with a great deal of experience in terms of my future research activities.

4．Acknowledgements

　I would like to express my sincere gratitude to ZEON Corporation members for accepting me for this two-month long internship. I would like to thank Dr. Ono, Mr. Shirota, and everyone at the R&D Center for their support in many ways, not only in proposing and discussing themes, but also in providing us with various opportunities to interact with each other. I also had many opportunities to receive advices from various people, which made the time that I spent with them very meaningful. I would also like to thank Mr. Tsunogae and Mr. Aoki for their assistance with various administrative procedures.

　I would like to thank again all the people involved in this internship.