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Experience, Data-Driven and Artificial Intelligence in Social (Fire) and Chemical Technology

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Abbreviations: AI-Artificial Intelligence, ICT-Information and Communications Technology.

Introduction

"Realization of society 5.0 in fire and disaster prevention activities" is one of intensive goals of Japanese government developing fire technology [1]. Improvement of new equipment and materials for disaster response utilizing AI and ICT should be developed according to social requirements. Efforts to predict earthquake, pour, flood, etc. through AI analysis of data collected from past disasters must continue. In parallel with such elaboration of disaster prediction, it is necessary to proceed with preparations for prompt and accurate provision of disaster information during emergency situations and support for rebuilding lives post disaster.

Discussion

Recently, Spring-8 (large synchrotron facility in Japan) has developed a program "Deep Centering" that automatically detects protein crystal samples in X-ray crystal structure analysis by image analysis using deep learning [2]. The result of this research realizes automatic positioning of protein crystals and is expected to be applied to fully automatic data collection and automatic structural analysis. In X-ray crystal structure analysis, a crystal centering is carried out position the sample crystal in the X-ray optical path irrespective of direction of rotation. Conventionally, this work is carried out mainly by the user of the beam line or by detecting the position of the crystal by irradiating the crystal with a weakened X-ray. This has made it possible to save labor and avoid radiation damage caused by X-ray.

According to bad examples reported by Akitsu [3], the normal procedure for manually centering a single crystal is described as follows. Firstly, a single crystal is attached to move sideways so that the center of the single crystal overlaps the center line (usually toward the center) in the direction seen with the microscope. Now axis is rotated (Φ) 180 degrees. So, in the direction being looked at the microscope, it is moved sideways so that the center of the single crystal overlaps the center line (usually towards the center), and repeat several times (but many times due to vertical misalignment).

Then, axis is rotated (Φ) 90 degrees. Therefore, in the direction being seen with the microscope, the single crystal is moved sideways so that the center of the single crystal overlaps the center line (usually toward the center). And axis is rotated (Φ) 180 degrees. Therefore, in a direction as viewed with a microscope, the lateral movement is repeated several times so that the center of the single crystal is overlapped the center line (usually toward the center).

Finally, axis is rotated every (Φ) 90 degrees to be confirmed that the center of the single crystal is overlapped the center line. In this way, the final "correct" position is assumed to be on the inner side than the initial state (the normal deviation is maximized), and the deviation from the center line of the single crystal is adjusted to be smaller.

If the center of the single crystal is shifted from the aiming center line from the beginning. Which is difficult to be aligned the center position by this method only by rotating the Φ axis. *Although I have read the APEX manual by the Department of Chemistry at Purdue University, where Dr. Negishi was awarded the Nobel Prize in Chemistry, there was a figure very similar to that "Asahi Beer's object" on P11* [4-6]. Figure 1, however, exhibits terrible example of failure alignment by a "novice" in my group.

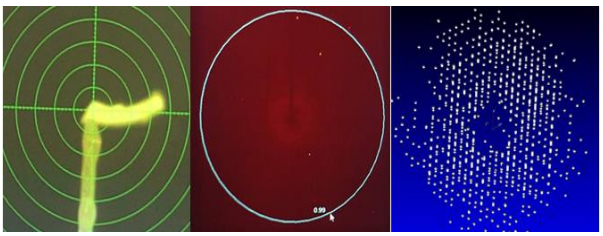

Figure 1: Failure of single crystal experiments; [left] Bad alignment, [middle] Poor resolution, and [right] unusual data.

Conclusion

Even though researches based on data are good at interpolation, it is said that prediction beyond experience is not good. In particular, in Japan, there are many excuses for "out of scope" (Sotei-gai in Japanese) when accident or disaster occur actually. *Therefore, I think what I have done after seeing immature's Sotei-gai poor experiments*.

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