Report for the internship

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Company	Nissan Arc Co., Ltd.
Training department	Device analysis unit
Practice period	June 4th, 2018 ～July 27th, 2018
Theme	Application and introduction of classical MD technique on mechanical analysis of engineering plastic.

Background

Because polyamide is comparatively easy to synthesize and robust, polyamide is one of the five major engineering plastics and are widely used industrially. For example, nylon 6 and 6,6-nylon are highly stretchable as fibers, and are widely used as materials for clothing articles. Polyamide 12 is excellent in impact resistance and durability, and in form of resin it is used in the automobile and aerospace industries.

Application examples of polyamide 12 (PA 12) as a gas pipe also exist. Since the inside of the gas pipe becomes under high pressure, durability is required. However, the mechanism of toughening at the molecular level in polyamide resins has not been elucidated, and there is still room for toughening in PA12 gas pipe at the stage of molecular design and molding processing.

Therefore, in this internship, for the purpose of elucidating the toughening mechanism of PA12 requested from a certain company, mechanical properties of PA 12 resins are calculated, using the classical molecular dynamics (MD) method which I normally use in research.

Research contents and results

From the results of preliminary experimental analysis, it has been known that specimens with higher degree of crystallinity are more brittle and harder but more durable, and as a result of discussions, it was hypothesized that the degree of crystallinity influences this mechanical property, and is influenced by the molding process of the material.

Therefore, in order to verify this hypothesis, this internship divided the goal of internship into two stages. First, we created a full-atomic MD model that reproduces the glass transition point, which is an important index for evaluating the physical properties of plastics. Subsequently, by applying the model, a model of polyamide with different degrees of crystallinity was prepared and the mechanical properties were evaluated.

To set initial coordinates of the molecule, I learned how to use the software used in Nissan Arc, and to convey MD calculation, I used cluster machine which Nissan Arc have, and open source molecular dynamics simulation software which I normally use.

First, about glass transition point, models of PA 12 was prepared using two force fields, the system was gradually cooled from high temperature, and the transition point in volume was defined as glass transition

point. As a result, in one forcefield, the calculated value was reasonable comparing to literature value. Similar calculations were made on polyamide 6, 6,6-nylon and polyamide 11, and the glass transition point was reproduced well in the same way.

Subsequently, similar cooling process was performed by changing the cooling rate to prepare two PA 12 bulk models with different degrees of crystallinity. The uniaxial elongation simulation was carried out using the model created. As a result, the tensile stress yield seen in plastics was reproduced by calculation, and the relationship between crystallinity, hardness and brittleness / ductility agreed with the results of preliminary experimental results. The slower the cooling rate, the higher the degree of crystallinity is, the harder and brittle PA12 becomes. Conversely, the higher the cooling rate, the lower the crystallinity is, and the softer and ductile PA12 becomes.

Also, through this internship, I was able to introduce the MD simulation technique for polymeric materials that Nissan Arc have not been able to handle until now.

Impression

What I felt most meaningful in my internship was that I was able to learn how I can contribute to industry and human society by using my research technique. The department to which I was assigned has a lot of employees with Ph. D. in particular, so I could see the active employment of their specialty, which became a very good stimulus, and so I was able to find out how to utilize my specialty.

In addition, I was able to experience a series of flow of analytical company tasks from client's request to construction of solutions using experiments and calculations. In addition, I could see how to manage time in companies and how to take consensus within the team, and I was able to obtain many knowledge that can be utilized in future research life.

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