Multiscale Simulation for Polymer Material Design

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Polymer materials such as plastics, rubber and fiber are widely used for industrial products. Not only conventional bulk materials, polymer materials also used in many high-tech materials such as electric devices, battery and artificial organ, and various kinds of function are required for each product. Such functions and properties are controlled by the structure of polymers, and main objective of polymer material design is to design the structure of polymers and to predict the properties of the materials from the structure.

However, the structure of polymers includes very wide range of length scale and time scale. For example, chemical structure of monomer unit is a finest structure of polymers. On the other hand, crystalline structure and phase separated structure are examples of larger structure. Since the polymer structure includes such a wide range of scale, multi scale and multi physics modeling is necessary to design polymer materials.

We will introduce a simulation platform for soft material, OCTA (Open Computational Tool for Advanced material technology). The OCTA was developed in a national project of Japan, then the OCTA was opened for the public after the project finished (available from the website, http://octa.jp/). From the release of the first version of OCTA in April 2002, it has been maintained by many people and the more than 1000 sites became users of OCTA. The concept of OCTA is shown in Figure 1. The OCTA contains several simulation program (Engine) and user interface (Platform). Each engine is based on different physical models, and covers different length scale and time scale. Furthermore, collaborative operations between engines are conducted to obtain realistic structure and properties of soft materials.

The OCTA project was thought to be succeeded as a first step, but we still need to enhance the science and technology to conduct multiscale modeling, which truly contribute the polymer material design in industry. We will present the success and the problems to be solved in the future.

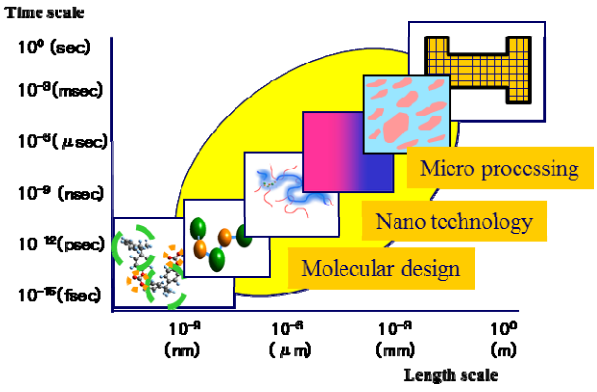

Figure 1. The concept of OCTA