【Grant-in-Aid for Transformative Research Areas（B）】

Section II

Title of Project： Precision Degradation of Polymer and Polymeric Material

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Number of Research Area：20B203　Researcher Number：40584529

【Purpose of the Research Project】

Polymer materials such as plastics are used in a wide range of material fields due to their excellent physical properties and processability. The decomposition of polymeric materials during or after use causes serious problems in various usage environments. Generally, it is still difficult to predict the polymer decomposition precisely, partly due to the lack/delay of systematic research on the decomposition of polymers. Simultaneously, it is not easy to suppress deterioration and decomposition and improve the stability of polymeric materials. These problems are because the decomposition of macromolecules has not been understood in multiple layers from the macro-level to the molecular level via the mesoscale. Despite the demand for polymer design based on theoretical prediction of stability and degradability of polymeric materials in various fields, it has not been realized due to the lack of systematic research on polymer decomposition and degradation.

This research project aims to clarify the degradation mechanism of polymers and polymeric materials with considering the hierarchical structure in terms of physical deterioration, chemical decomposition, and biological degradation and metabolism. Furthermore, the long-term goal is to provide new polymer design guidelines that consider degradability and environmental impacts. For the molecular theory that experiments cannot approach, the level of coarse-graining is judged based on the information obtained from the experiments, and computational science is introduced to clarify it.

【Content of the Research Project】

This research project promotes four planned research topics and two fusion research subjects to construct a theory and guideline that enable the precise decomposition of macromolecules and macromolecular materials. The planned research includes “A01 Elementary process of physical deterioration using uniform polymer network (physical deterioration)”, “A02 Precise design and time-course analysis of polymer chain cleavage under usage environment (chemical decomposition)”, “A03 Precise characterizations of degradation products and evaluation of their impact on the biological environment (biological metabolism)”, and “A04 Polymer decomposition simulation by effective coarse graining (decomposition prediction)”. Through these planned studies, we will consistently study physical destruction processes such as deterioration and wear of polymer materials, chemical polymer chain breaks, and decomposition products and their effects on living organisms in nature. Computational science will promote the phenomena that are difficult for the experimental evaluations. At the same time, by linking the four research topics, this research project sets two fusion research subjects, namely, “P1: the theory of spatiotemporal effects” and “P2: the theory of homogeneity and heterogeneity”. P1 promotes research on polymer decomposition effects, focusing on its time scale and spatial scale, that is, the degradation rate and degradation product concentrations. In P2, we approach the precise decomposition of polymers based on the presence or absence of a hierarchical structure of macromolecules, that is, the homogeneity and heterogeneity in the structure.

As pointed out in the reviewers’ comments on our project application, there is a risk of dissipating research results due to the wide scope of this project. Thus, we decided to focus on rubber polymers that are feared to impact the natural environment as well as biodegradable thermoplastic (polyesters) as the main target polymers in this research project according to discussions in the kick-off symposium.

【Expected Research Achievements and Scientific Significance】

When this project is achieved successfully, we will be able to design and synthesize the polymers with precisely designed and controlled degradability, such as polymers that are safe to leak into the natural environment, biomaterials that can be safely used *in vivo* for a long time, and closed-loop recyclable polymer materials.

【Key Words】

· Polymer materials: Human life is made up of many polymer materials including rubber, plastics, synthetic fibers.

· Precision decomposition: Although research on the precision synthesis of macromolecules has been carried out for many years, the precision decomposition theory that systematically controls the decomposition process is insufficient so far.

【Term of Project】 FY2020-2022

【Budget Allocation】 122,100 Thousand Yen

【Homepage Address and Other Contact Information】

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