【Grant-in-Aid for Scientific Research (S)】

Broad Section E

Title of Project : Development of new fabrication methods of polymer materials based on the structurally controlled hyperbranched polymers

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【Purpose and Background of the Research】

Synthetic polymers are now indispensable materials for maintaining the QOL of modern society, and the demand for their further improvement is never-ending. On the other hand, the inherent advantages of synthetic polymers, such as low cost, high stability, and good processability, have become the origin of waste plastic pollution. Solving these issues has been an urgent issue in polymer chemistry. We focus on structurally controlled hyperbranched polymers (HBPs), providing solutions to both of the issues.

While structural control and practicality have been in a trade-off relationship in HBP synthesis so far, our group has recently developed a new practical synthetic method of structurally controlled HBPs using controlled radical polymerization. Since this method has a living polymerization property, the growing chain-end can be converted into various functional groups. Thus, we aim to create functional polymer materials with self-healing properties based on the interaction of HBPs' end groups. We believe this formation principle would become a complementary method to the conventional one based on entanglement of linear polymer chains.

【Research Methods】

We will create next-generation synthetic polymer materials using the HBPs as key substances through the following four subjects; 1) creation of new HBPs by deepening the current HBP synthesis, 2) elucidation of structure, physical properties and functions of HBPs, 3) material development utilizing the characteristics of HBPs, and 4) database construction and machine learnings using AI. The specific plans are discussed below.

1) The HBPs with new branched structures will be synthesized by developing new initiators, and the structure control will be improved by optimizing the branching monomers and polymerization conditions. Furthermore, varieties of functional groups will be introduced to the HBP-ends (Fig. 1a).

2) The structure of the synthesized HBPs will be studied in a dilute solution using synchrotron small-angle X-ray scattering and light scattering measurements. Furthermore, the dynamics of the interaction of HBPs in bulk will also be studied.

3) Functional polymer materials using unimolecular and bulk HBPs will be developed. Self-healing materials will be targeted for the latter case (Fig. 1b).

4) An integrated database on HBP synthesis, structure, and function will be constructed. Furthermore, a tool for predicting the reactivity and physical properties of HBP synthesis will be created by carrying out the AI-based machine learning of the database.

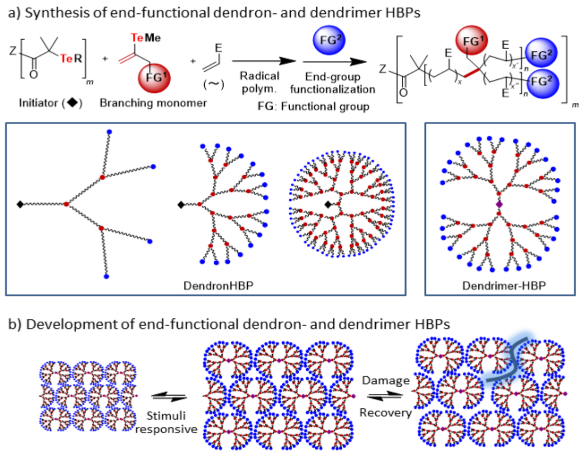

Fig. 1. Outline of research on HBP synthesis and development of functions

【Expected Research Achievements and Scientific Significance】

Basic principles for fabricating HBP-based polymer materials using the interaction of HBP's end-groups and an integrated database of HBPs will be established. The results will lead to the development of prototypes for the commercialization of HBP-based materials. In particular, improvement of functions including the self-healing properties is expected. New synthetic polymers with improved and/or new properties based on HBPs developed by this research will contribute to the realization of a safe and secure society and green innovations through providing highly functional and self-healing plastics.

【Publications Relevant to the Project】

- Yamago, S. "Practical Synthesis of Dendritic Hyperbranched Polymers by Reversible Deactivation Radical Polymerization", *Polym. J.* **2021**, *53*, 847-864.
- Lu, Y.; Nemoto, T.; Tosaka, M.; Yamago, S. "Synthesis of structurally controlled hyperbranched polymers using a monomer having hierarchical reactivity", *Nat. Commun.* **2017**, *8*, 1863.

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