Development of Multi-Lock Biopolymers Degradable in Ocean From Non-Food Biomasses

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AIST (National Inst. Advanced Industrial Science and Technology)
Research and development of multi-scale analysis methods for marine degradable polymers from a hierarchical point of view

MOONSHOT RESEARCH & DEVELOPMENT PROGRAM NEDO

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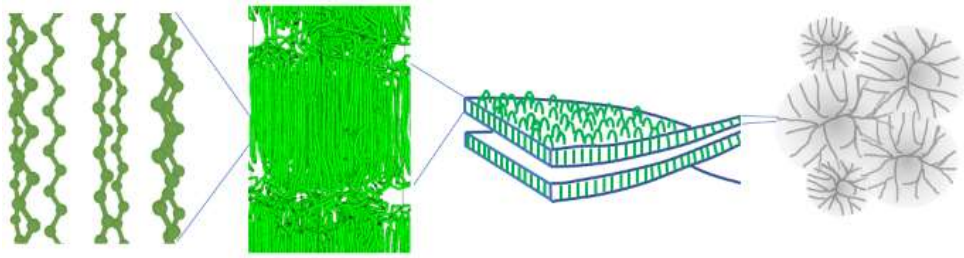
Our group tackle the issues of the marine degradable polymers treated in this project using our advanced technologies of simulation and informatics. Using those technologies, analysis and material designs of marine degradable polymers in multi-scale are performed.

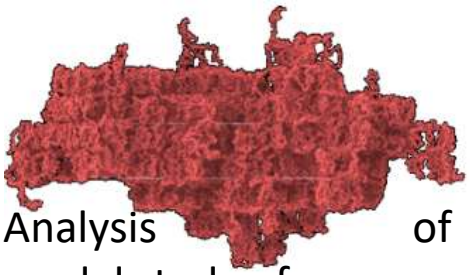
In our group, we studied two kinds of topics of marine degradable polymers; 1) Model study of degradation process of polymer crystals, and 2) Model study of degradation of multi-locked polymer. In first topic, we modeled the polymer crystal structure using coarse-grained technics and performed the degradation process simulations induced by heat with precise analysis of structures based on machine learning. In the latter topic, we made the simulation models of dynamic cross-link elastomer having multi-lock functions and performed the simulations to analyze the detail of dynamic cross-link process. From our simulation and informatics studies, we will try to design the marine degradable polymers having multi-locks.

Hierarchical structures of polymeric materials

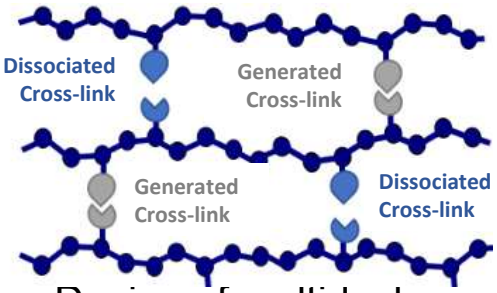


Simulation + informatics

Analysis and material designs of marine degradable polymers.



Analysis of model study of degradation of crystal



Design of multi-lock functions in polymer

AIST

E4a: Research and development of multi-scale analysis methods for marine degradable polymers from a hierarchical point of view

Strong points of our group

- Multi-scale simulation techniques of polymeric materials.
- Analysis of materials using informatics techniques

(2029 FY) Final objective

・Our group perform the development of material design from the hierarchical point of view and proceed the combined modeling in several scales. Along this procedure, the united design method of marine decomposition polymer in multi-scale will be achieved, and the analysis of degradation of marine plastics using coarse-grained simulation will be realized.

・Our group will propose the conditions with better decomposability in the parameters such as the material parameters related to multi-lock functions or process parameters related to degradation of marine plastics. Through the collaboration with members of E1 and E3, we will contribute to design and develop the marine degradable multi-lock polymer having the targeted functions of degradation.

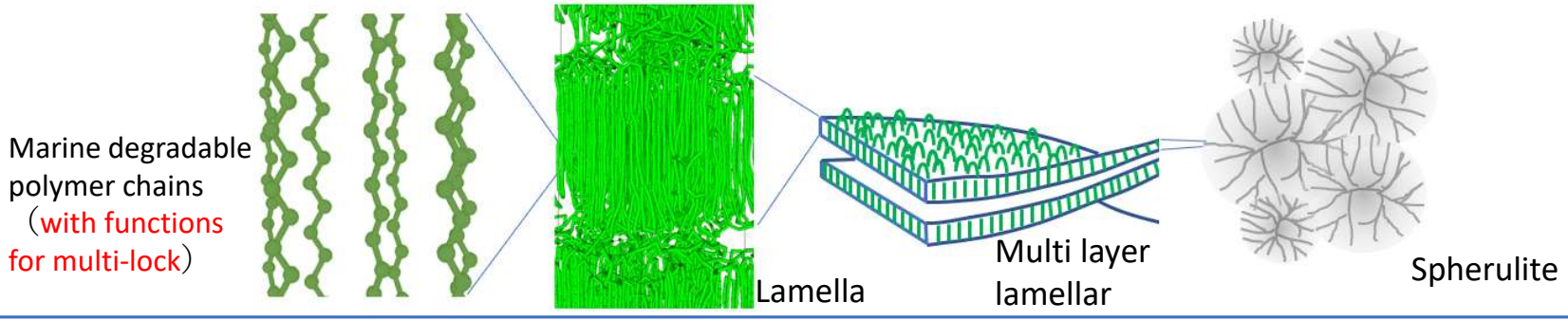
Objective until 2021 FY.

・Model study of degradation process of polymer crystals: We perform the modeling of polymer crystals and perform thermal decomposition simulations of polymer crystals. Collaboration with experimental analysis group in E2 Group will be examined.

・Model study of degradation of multi-lock polymer: We will build a coarse-grained molecular model for multi-lock polymers to be developed at each of the E1 and E3 groups as candidate materials for marine degradable biobased tough polymers. Specially, we treat the multi-lock polymers applicable for rubber materials and perform the simulation to observe the degradation of those polymers.

Items of our research works

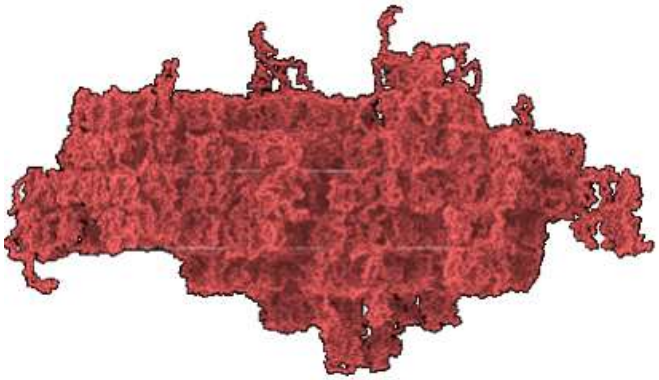
Hierarchical Structures of polymeric materials



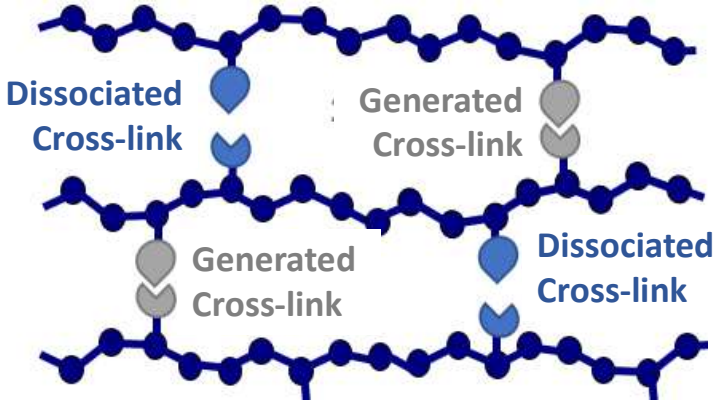
Simulation and informatics techniques

Our study: Analysis and material design for marine degradable polymer with multi-scale problems in polymeric materials

Items of our studies



Analysis of model study of degradation of polymer crystal



Design of multi-lock functions in polymer

Current status 1

Objective：Major parts of marine plastics have polymer crystals.

⇒ Development of Multi-lick functions effective to marine degradation of plastics

Analysis of mechanism of marine degradation and its probability.

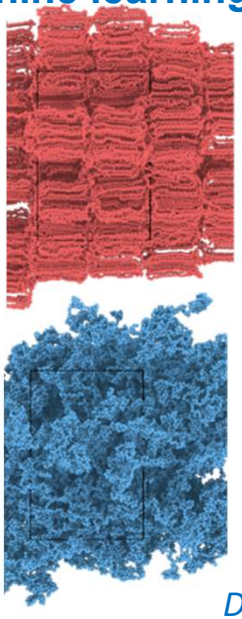
（trigger affected to multi-lock: heat, sun light et al.）

Our research plan：

・Degradation simulation of polymer crystal based on coarse-grained model.

・Detail and quantitative analysis of crystal parts in degrading polymers

Analysis of local structure using machine learning.



$o=$ lamella

$D_{lamella}$

$o=$ melt

D_{melt}

Machine learning

$$\boldsymbol{o} = D\boldsymbol{w}$$

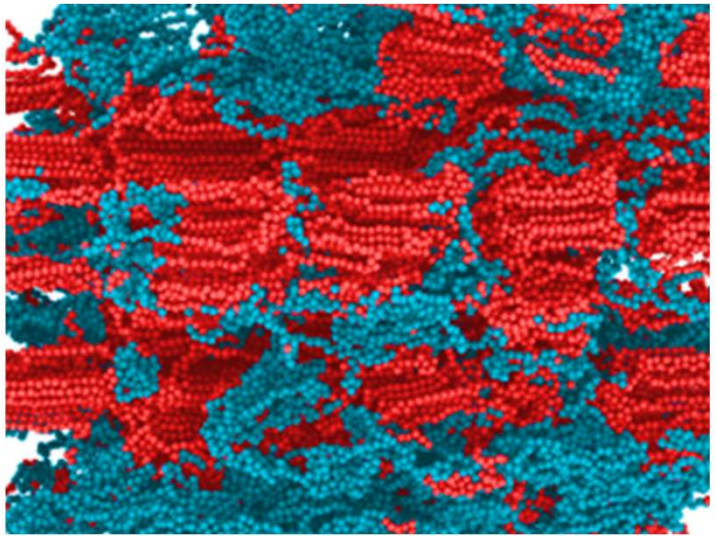
$\boldsymbol{w}$ ： optimized by learning

o: objective variable

D: explanatory variable (Those are obtained from structural motifs.)

Applied

Analysis of fine structures in heat degradation simulation



Classification of crystal and melting parts using machine learning on the results of heat degradation simulation. （Red：crystal part、blue：melting part）

Current status 2

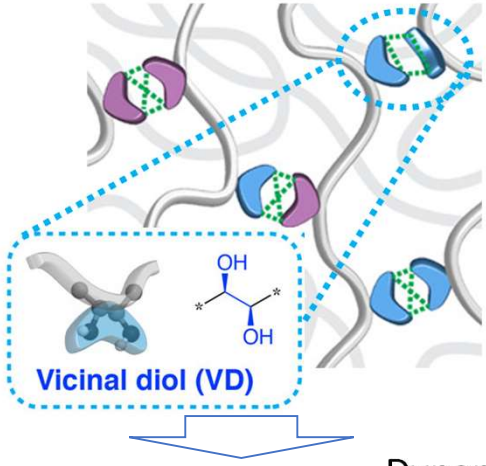
Objective ：Development of marine degradable multi-lock bio-polymer by E1 and E3 G.
⇒Design of polymers having toughness and marine degradability using multi-locks.

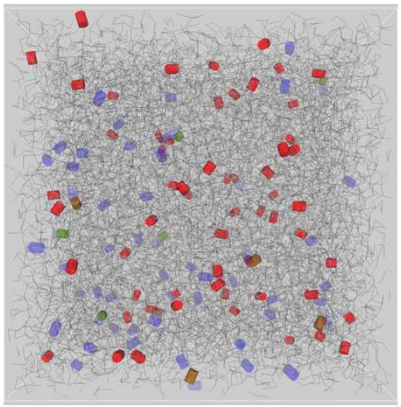
Our research plan ：

・Modeling and simulations of dynamic cross-linked elastomers developed by Yoshie group (E1).

・Analysis of features of cycle deformations and self-healing on our simulations.

Modeling of dynamic cross-linked elastomers



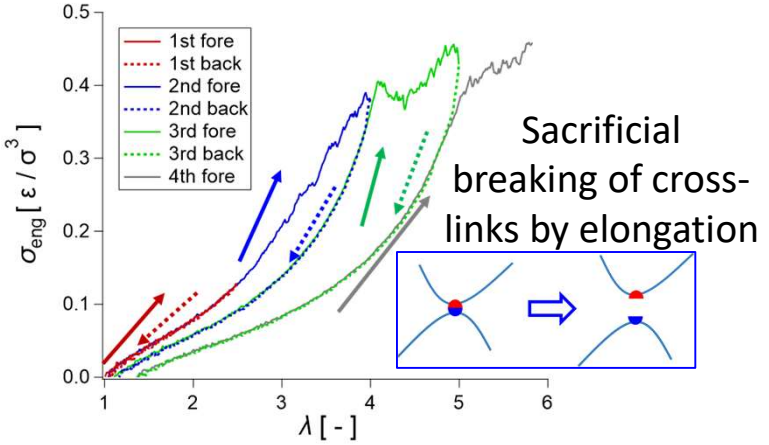


Dynamic cross-linking is realized in simulations.

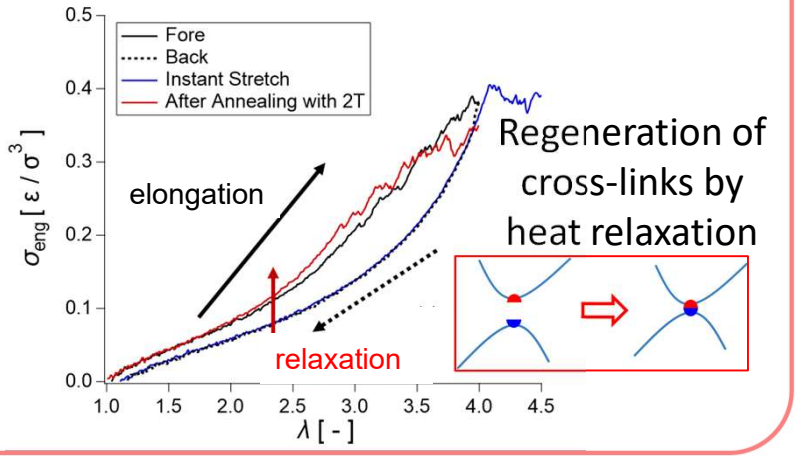
Gray：Network
Red： Generated bond
Blue： Dissociated bond

Properties of dynamic cross-linked elastomers

Under the generation and dissociation of dynamic bonds, we can reproduce the fracture resistance in the high elongation region.



By thermal relaxation, the stress could be recovered, and the self-healing property could be reproduced on the model.

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