The University of Tokyo

Molecular Dynamics Simulation Study of Multi-Lock Biopolymers and Development of Data Base of Polymer Dissociation and Fracture

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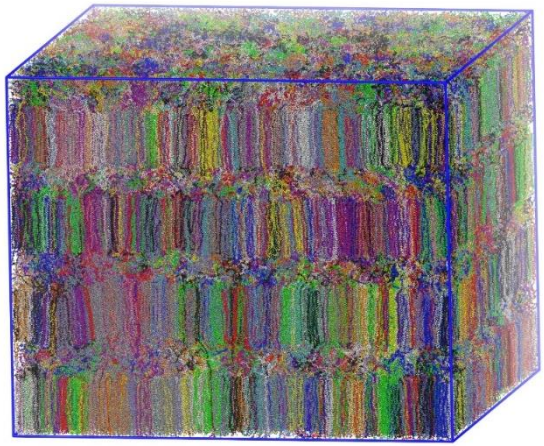
1. Fracture Mechanism of Crystalline Polymers
Molecular mechanism of elasticity, yielding, and fracture of biodegradable crystalline polymers is investigated based on all-atom molecular dynamics calculation. In particular, we focus on lamella structures in polycaprolactone (PCL). Change in mechanical properties of amorphous region of crystalline polylactic acid (PLA) caused by water molecules is also investigated.
2. Dissociation Mechanism of Double-Lock Polymers
Electronic mechanism of dissociation of double-lock polymers by metal cluster catalysts is investigated based on quantum chemical calculations. Light and sea water opening the double locks on the polymer dissociation are investigated in detail.
3. Data Base
Data base archiving dissociation and fracture properties of polymers is developed. Input tool can produce tagged tree-type meta-data which enables systematic search of the data. The data base will be managed on NIMS PDF and served for machine learning studies.

Number of molecules：9,900,825
Degree of polymerization：2000
Number of chains：275
Periodicity：10 nm
Thickness of the lamella：7 nm
Thickness of amorphous phase：3 nm



A lamella structure of PCL constructed by 10 million atoms.