

# パーシステントホモロジー解析を用いた高分子材料の 強度と構造の解析

## The Persistent Homology Analysis for Strength-Structure Relationship for Polymer Materials

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### Abstract

Controlling the mechanical properties of polymer films is crucial for ensuring the robustness and stability of waterborne paints. However, due to the complex structures of polymer films, it is not straightforward to directly correlate mechanical properties with atomic-scale polymer structures. In this tutorial paper, we introduce a method recently reported by the authors that correlates polymer film structures with stress-strain curve using persistent homology analysis (R. Sato *et al.*, *J. Chem. Theory Comput.*, 20 (2024) 10798). In this approach, the time evolution of atomic coordinates during the uniaxial tensile simulation was analyzed, successfully predicting the shape of the stress-strain curve without using any prior knowledge about mechanical properties. Furthermore, inverse analysis of persistence diagrams allows the extraction of polymer structures corresponding to changes in the stress-strain response. The results demonstrate that specific ring structures play a key role in determining stress-strain behavior. These ring structures were consistent with those inferred from the potential form of polyethylene oxide used in these simulations, indicating that a physically reasonable picture was obtained. Overall, this method provides an effective framework for understanding the relationship between polymer film structures and their mechanical properties.

キーワード：ポリマーフィルム、応力-歪曲線、パーシステントホモロジー解析、分子動力学計算  
**Keywords**: Polymer Film, Stress-Strain Curve, Persistent Homology Analysis, Molecular Dynamics Simulation

2025年12月24日受付

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### 1. はじめに

塗料材料であるポリマーは、産業分野において広く用いられている。従来の溶剤系塗料では、揮発性有機化合物 (VOC) による環境負荷や健康リスクが問題とされてきたが、水を主溶媒とする水性塗料はこれらの課題を大幅に低減できる。そのため、環境規制の強化を背景として、