Analysis in structural features of polymer systems by persistent homology

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Polymer is made up of monomers that are repeating structural units to form a long chain structure. As a result of its snake-like form, polymers flexible move and deform, which can be curled, elongated, and tangled. Thus, the polymer system, called soft matter, involves various local structures and unique responses because of the structural features of polymers. Our question is how polymers are becoming loose or entangled depending when the system deforms. As a first step, we investigate structural features of facture process of a polymer system using persistent homology. The fracture process of a polymer system is examined by molecular dynamics simulation in three dimension. At first, a condensed polymer system is in an equilibrium state. After stretching whole system in one direction, polymers are clearly elongated and finally the system is almost fractured. The polymer system contains different local structures at the initial state and the finial state. However, the detailed structures in three dimension is hard to distinguish because of its complexity. Thus, we use persistent homology, which is an algebraic tool for systematically characterizing geometric objects. Persistent homology can capture the topological properties such as rings and cavities, and provide the metrics of these topological properties. In recent years, persistent homology and its graphical representation, persistent diagram (PD), can be computed efficiently. Some types of condensed systems are well distinguished its local structures using persistent homology and PDs [1,2,3]. As a first test, we analyze the configurations of polymers of the initial and final states using the persistent homology. It successfully distinguishes a difference of local structures. For example, the system in the final state contains larger and more elongated pores comparing with those in the initial state. In addition, there are small structures which are kept during the fracture process. Persistent homology may shed light on a structural feature of fractures of a polymer system. In this talk, we will introduce persistent homology and structural features of polymers in a fracture process.

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