Topological approach to pattern formation problems arising in materials science

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Topological approach is a new non-invasive mathematical measurement potentially applicable to various fields including materials science. In this talk I will present two case studies in which computational homology and its variants play a key role to extract essential information on morphological dynamics arising in materials science.

One is the diblock copolymer problem in a three-dimensional space. It is known that the double gyroid and orthorhombic morphologies are obtained as energy minimizers. By investigating the geometric properties of these bicontinuous morphologies, we demonstrate the underlying mechanism affecting the triply periodic energy minimizers in terms of a balanced scaling law. Then we apply computational homology to characterize the topological changes during the morphology transition in three-dimensional space. It should be noted that even the “transient” morphologies can be detected during the time course of the transition, since integer-valued index (Betti numbers) can be observed for certain time before reaching the final state, for instance, transient perforated layers are found from layers to cylinders. The scaling law for Betti number in the phase ordering process is also presented.

The other study is about the bulk metallic glasses (BMGs). BMGs have been extensively studied because certain mechanical properties, such as strength, can be significantly improved over their crystalline counterparts. Although BMGs are metallic alloys, they do not have crystalline structure nor random one. Numerous rules, criteria, and mechanisms have been proposed to guide the development of metallic alloys with high glass-forming ability (GFA), however there is no general principle characterizing the basic features of BMGs. For instance, it is known experimentally that the best glass former in an alloy system is located at a pinpoint composition for two component alloy like Cu-Zr. The existing mechanisms and criteria for glass formation fail to explain why the best glass former only occurs at a pinpoint composition. The atomic-level microstructure of metallic glasses is a long-standing subject that has been attracting large interest. Although the atomic structural picture is far from being established, it has been realized that clusters should be the building block in glassy alloys. I will present a progress report on the issue of pinpoint composition by using the persistent homology, especially focusing on the topological characterization of such a pinpoint.

The first part is a joint work with T. Teramoto (Asahikawa Medical University) and the second one is with A. Hirata (WPI-AIMR, Tohoku Univ.) and his collaborators.