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PRESS RELEASE (2024/12/03)

Dynamics of structural transformation for liquid crystalline blue phases

Researchers explore the transformation dynamics of cubic liquid crystals using direct simulation and machine learning, offering new possibilities for advanced materials development

Fukuoka and Tsukuba, Japan—Researchers have uncovered key insights about how liquid crystals, materials capable of forming complex ordered structures, transform between different phases. **Published in *PNAS*,** the study provides a clearer understanding of how these materials change their structures at the microscopic level. This research could provide a means to give a deeper insight into the transformation between different structures in a wider variety of materials.

Liquid crystals are materials that exhibit properties of both liquids and solids. They flow like liquids but can also form ordered structures like solids. Liquid crystals are widely used in devices such as digital displays, light-responsive materials, and sensors. However, despite their widespread use, understanding how they reorganize at the microscopic level has long been a scientific challenge, and the underlying mechanisms have remained unclear.

Professor Jun-ichi Fukuda from Kyushu University's Department of Physics, in collaboration with Dr. Kazuaki Z. Takahashi from the National Institute of Advanced Industrial Science and Technology (AIST) and the Japan Science and Technology Agency (JST), performed a study focusing on cholesteric blue phases, a specific type of liquid crystal characterized by its unique cubic symmetry. These blue phases form complex three-dimensional structures with distinctive properties, making them a subject of great interest in both basic science and materials engineering.

The team investigated the transition from one blue phase, BP II, to another, BP I. As BP II changes into BP I, the liquid crystal forms twin boundaries—regions where two parts of the material align differently. Previous experimental studies fail to capture the detailed mechanism of transformation of blue phases involving the formation of twin structures.

To gain a deeper understanding of this process, the team employed computer simulations performed by Fukuda, and MALIO, a machine learning tool Takahashi designed to analyze and distinguish the local structures of BP I and BP II liquid crystal phases. The exploitation of the latter machine learning approach makes it possible to distinguish between the BP II and BP I structures, and to analyze their evolution over time. The strategy developed by the team allowed the tracking of the transformation in real time, revealing key stages in the transition such as the formation of small BP I domains, which grow and eventually form twin boundaries. Their approach provides valuable insights into the formation and growth of twin structures during the transformation.

"The dynamics of soft materials like liquid crystals are highly complex," says Fukuda. "This work has given us a deeper understanding of how these materials transform at a microscopic level."

The approach presented in this study could also reveal how hierarchical structures in soft materials, such as polymers and biological systems, undergo similar phase transitions. "Our method is not limited to liquid crystals," Fukuda explains. "It can be applied to other complex materials, which can offer new insights into how structures form and change in systems."

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For more information about this research, see "Direct Simulation and Machine Learning Structure Identification Unravel Soft Martensitic Transformation and Twinning Dynamics", Jun-ichi Fukuda, and Kazuaki Z. Takahashi, *PNAS*, DOI:
https://doi.org/10.1073/pnas.2412476121

About Kyushu University
Kyushu University is one of Japan's leading research-oriented institutes of higher education since its founding in 1911. Home to around 19,000 students and 8,000 faculty and staff, Kyushu U's world-class research centers cover a wide range of study areas and research fields, from the humanities and arts to engineering and medical sciences. Its multiple campuses—including one of the largest in Japan—are located around Fukuoka City, a coastal metropolis on the southwestern Japanese island of Kyushu that is frequently ranked among the world's most livable cities and historically known as Japan's gateway to Asia. Through its Vision 2030, Kyushu U will 'Drive Social Change with Integrative Knowledge.' Its synergistic application of knowledge will encompass all of academia and solve issues in society while innovating new systems for a better future.

About AIST
The National Institute of Advanced Industrial Science and Technology (AIST), one of the largest public research organizations in Japan, focuses on the creation and practical realization of technologies useful to Japanese industry and society, and on "bridging" the gap between innovative technological seeds and commercialization.
For this, AIST is organized into 5 departments and 2 centers that bring together core technologies to exert its comprehensive strength.
AIST, as a core and pioneering existence of the national innovation system, has about 2300 researchers doing research and development at 12 research bases across the country, based on the national strategies formulated bearing in mind the changing environment regarding innovation.
AIST is also actively building a global network by, for example, signing memorandums of understanding for comprehensive research cooperation (MOUs) with major research institutes around the world.

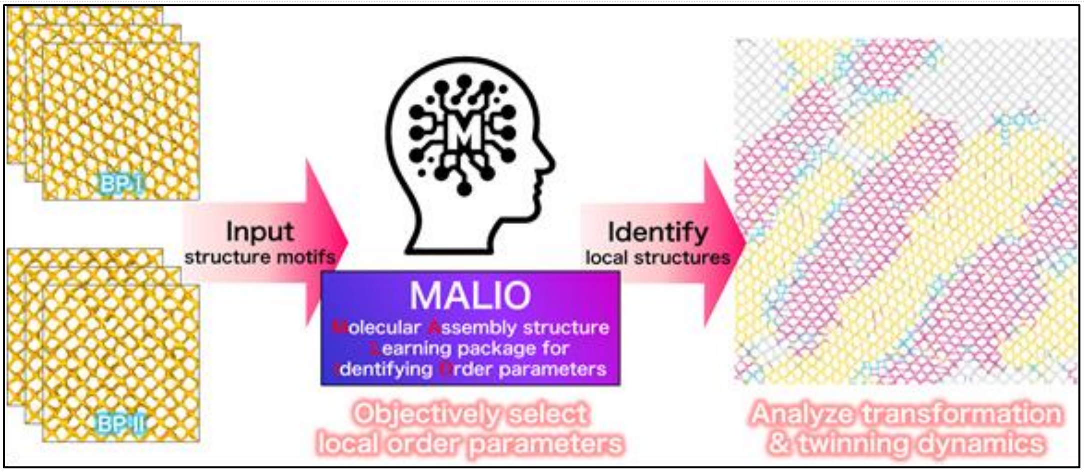

Fig. 1. Machine learning-based analysis of BP I and BP II liquid crystal structures. This schematic illustrates the MALIO software, a machine learning structure analysis tool designed to analyze and distinguish the local structures of BP I and BP II liquid crystal phases. By processing input motifs, MALIO identifies the best local order parameters, enabling accurate differentiation between these two phases. This, in turn, enhances our understanding of liquid crystal phase transitions and their structural properties. (Kazuaki Z. Takahashi, AIST, Japan)

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