【Grant-in-Aid for Transformative Research Areas（B）】

Rheology of disordered materials: Establishing Anankeon dynamics

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Purpose and Background of the Research

●Outline of the Research

The demand for materials industry to discover new materials and to enhance the functionality of existing materials is becoming more acute, requiring the development of functional materials with complex structures that exhibit excellent characteristics. Controlling structurally disordered materials, such as liquids and glasses, in which atoms and molecules are randomly arranged, is one of the strategies for the fabrication of new functional materials. As shown in the figure 1, there are a wide variety of disordered materials in a wide range of length scales. In order to realize high performance, high functionality, and control of these materials, a new research field, different from solid state physics established at the beginning of the 20th century, is required to be created. That is, "**the science of structurally disordered systems**. Because of the absence of long-range order, disordered systems have no solid structures. Therefore, they show a variety of mechanical responses to external forces. Accordingly, the science of disordered systems aims to understand the origin of rheological properties, such as softness and ease of flow due to irregular structures. However one has not yet developed a sufficient theory to meet social demands, and it has not been established as an academic framework covering from basic to applied sciences.

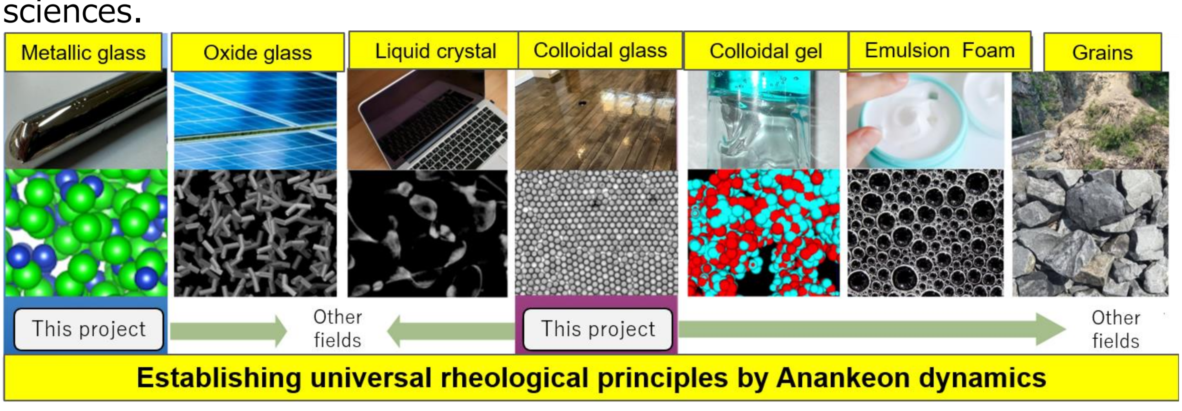

Figure 1. A disorder material is important for a wide variety of materials on a broad range of length scales.

The problem essentially lies in the irregularity of its structure. For disordered material, structural irregularities such as lattice defects in crystals are not easily discernible. Therefore, it is not possible to clearly identify what plays an important role in the expression of their rheological properties. Here we considered the following reason for this problem that many existing studies on structurally disordered systems were based on the paradigm that "the structure of a material can predict its physical properties," a concept that had been developed in solid state physics. The conventional approach of scrutinizing static structure of irregular structures is itself very useful in that it allows understanding and predicting thermodynamic, vibrational, and electrical properties. However, targeting a static structure cannot realize the prediction of dynamic properties, i.e., rheological properties, of structurally disordered systems. In order to truly understand the mechanical properties of structurally irregular materials, a shift in thinking **from "static to dynamic"** is required.

In collaboration with the University of Tennessee and the Oak Ridge Laboratory, the project leader proposed that the elementary excitation governing the flow of liquid metals is the creation or annihilation of atomic bonds, named later as 『**Anankeon**』 (Fig.2). In terms of the change in interparticle interactions, their elementary excitations can be the key to describing a general deformation mechanism that is independent of specific materials and spatial scales. From this, we came to the conclusion that we can bring about an academic revolution toward a unified understanding of the dynamics governing structurally disordered systems by shifting the scientific paradigm **from "prediction based on static structures" to "prediction of based on dynamic structure.**

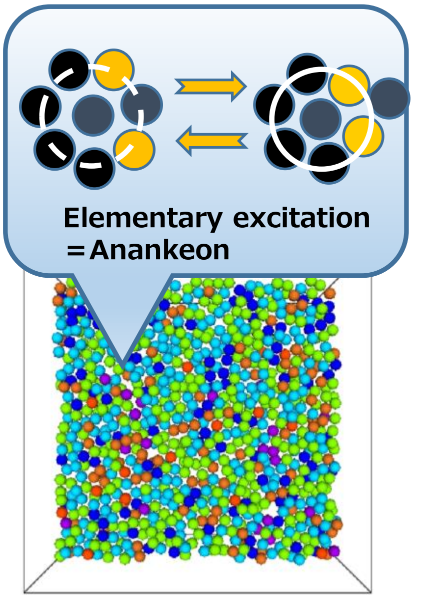

Fig. 2 Concept of Anankeon

Expected Research Achievements

The purpose of this research is to construct a unified theory on the spatio-temporal structure of dynamical elementary excitations (Anankeons) that can describe the macroscopic rheological properties of “metallic glasses” and “colloidal dispersion systems,” which are representative of structurally disordered systems.

- **Rheology of charged colloidal suspensions**

Colloid suspensions of charged colloidal particles in a solvent are known as functional fluids with complex response to external stimuli. In order to achieve high performance control, it is necessary to clarify the mechanism of viscosity that characterizes the ease of flow. Electroviscous rheology, in which the addition of a small amount of salt dramatically reduces the viscosity by more than four orders of magnitude, is a unique phenomenon that is ideal for linking viscosity and structural change. However it has been poorly understood. In this study, we combine computer simulations, rheological measurements, and small-angle X-ray and light scattering experiments to identify and quantify the conditions for the onset of dynamic structural changes, i.e., Anankeion, in charged colloidal suspensions.

- **Rheology of metallic glasses**

Metallic glass having disordered atomic structure shows novel mechanical property comparing with crystalline metals which have ordered structure. In order to expand practical use of metallic glass, improvement of their ductility is necessary. It is important to understand what kind of atomic structure causes atomic excitations (Anankeon), which governs plastic deformation of metallic glass. We previously revealed that mechanical work can give ductility to metallic glass, which means that the excitation of Anankeon became easier by mechanical work. This study aims to understand the atomic structure where the Anankeon excitation occurs by precise structural analysis of various metallic glasses having different activity of Anankeon excitations. We contribute to construct Anankeon dynamics from both experimental and computational perspective, which is the primary goal of this research project.

Ripple effects

There is no doubt about the emergence of interdisciplinary research through the development of numerous structurally disordered systems (oxide glasses, polymer glasses, colloidal glasses, granular solids, etc.) from this prototype project collaborating metallic glasses and colloidal suspension.

Homepage Address, etc.	https://www.anankeon.com/