【Grant - in - Aid for Scientific Research on Innovative Areas(Research in a proposed research area)】
Science and Engineering

Title of Project：Discrete Geometric Analysis for Materials Design

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Research Project Number: 17H06460　Researcher Number: 50230024

【Purpose of the Research Project】

Creating materials with outstanding functions supports our affluent life and can change our lifestyles and values. Japan is a world leader in materials science and industry, but creation of new materials is due to trial and error based on the experience and intuition of researchers and developers, and takes 20-30 years.

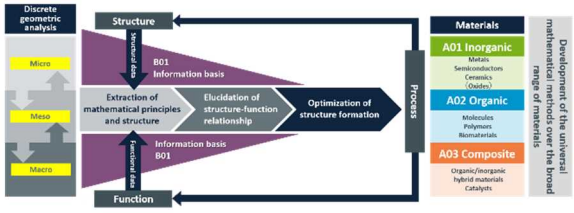
So major data-driven materials design projects applying information science have started in the US, Germany, China, etc. (e.g. Materials Genome Initiative). Computers use findings for search and classifying and material structures are screened for functional materials. But material structure and function correlations are complex, multiscale and involve multiphysics, so getting results with just information science is difficult.

To get meaning from masses of data, scientists must organize information with "good descriptors" that stimulate the imagination. A foundation for realizing and validating materials design is needed to describe layered structures intuitively and reveal the "structure, functions, processes correlation principle" that is key to material creation.

In this context we propose a universal and mathematical materials science through collaboration between mathematics and materials science in which Japan is strong.

【Content of the Research Project】

The aim is to understand the key structure, functions, processes correlation principle and develop geometric methods for that. We apply the latest findings of discrete geometric analysis to **disordered systems** and **multilayered hierarchical systems**, to clarify micro/mesoscopic structure and macroscopic property relationships, to change materials development from a **forward problem** to an **inverse problem**. We use discrete geometric analysis connecting discrete and continuous to find structures hidden behind diversity, and build a foundation for a unified understanding of complex materials.



Elucidating Process-Structure-Function relationship through network analysis of hierarchical structure of materials, especially by focusing on micro, meso, and macro structures (change from forward problem to inverse problem)

We work on the following research based on collaboration between mathematics and materials science.

- **A01 (inorganic): topological materials**
- **A02 (organic): polymeric materials using network analysis**
- **A03 (composite): dynamic structure formation of minimal surfaces and nano-structures**

In particular, we use discrete geometric analysis to **expand the unified theory from ordered to disordered systems (random and complex) and from static control to dynamic control**.

【Expected Research Achievements and Scientific Significance】

In academia the structure-function-process correlation principle is deepening, and new phase materials are being created using the power of information science and data science. In mathematics discrete geometric analysis and discrete dynamical systems that understand complex and multiscale structures hierarchically and study the correlation of discrete and continuous are making great progress. These contribute to materials development and human resources development for the big data society.

【Key Words】

Discrete geometric analysis: The discrete form of geometric analysis analyzing macroscopic geometric structure is discrete geometric analysis. The relationship of discrete and continuous is understood by developing a technique to find the continuous structure behind the discrete data.

Data-driven materials design: If conventional materials development is the forward problem of finding functions from structure, aiming to use data analysis techniques to solve the inverse problem of finding structures that have the required functions is data-driven materials design. It is also called materials informatics.

【Term of Project】 FY2017-2021

【Budget Allocation】 1,002,900 Thousand Yen

【Homepage Address and Other Contact Information】

https://www.math-materials.jp/