Research area in Strategic Objective *"Elucidation of macroscale mechanical properties based on an understanding of nanoscale dynamics"*

Elucidation of macroscale mechanical properties based on understanding nanoscale dynamics for innovative mechanical materials

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Overview

In this research area, we aim at the development of the technology to analyze and evaluate the motions of atoms and molecules in materials or on surfaces, the structural and chemical changes of microstructures, and other nanoscale dynamics. Thus, our purpose is to find the governing factors that determine the mechanical properties on the macroscale, to elucidate the mechanisms of their actions, and to find a principle or establish a guideline to design innovative mechanical materials with new mechanical properties in order to develop the material technology and to contribute to the realization of a society in which sustainable new industries are created.

Specific research areas include elucidation of new mechanical properties and the mechanisms of mechanical properties such as adhesiveness, friction, wear, deterioration, and destruction of the metal, inorganic, organic, and their composite materials as well as the development of the measurement and multi-scale simulation technologies on site for the visualization of the nanoscale dynamics and chemical changes on the nanoscale necessary for the abovementioned areas.

By integrating the knowledge acquired from the multilateral cooperation in each type of research area and from each type of material, such as metal, inorganic, organic, and composite materials, we construct a common scientific principle that is not dependent on the material types and elucidate the mechanisms of the mechanical properties of each material type or any specific material that has not been explained yet. In addition, we cope with the creation of guidelines of material design with new mechanical functions and the materials that break though the trade-off limitation in mechanical properties.

As already announced, JST and ANR invite Japanese-French joint research proposals, as well as regular (non-joint) proposals in FY2021.

Research Supervisor's Policy on Call for Application, Selection, and Management of the Research Area

1. Background

The primary material and machinery industries rank high to provide the most exported items of Japan: specifically, automobiles and their parts, semiconductors and other electronic parts, iron and steel, motors, plastics, and organic chemical compounds. While people want to embody a sustainable society, expectation is high for high-performance applications in these industries. However, people are now observing the limitation of Moore's law in the field of electronic device, and more limitations in the conventional design concept have been unearthed in each field.

Under these circumstances, to meet to the expectation of the society, we need to present a road map to innovate the conventional designing of machinery and equipment through the material innovation by developing high-performance/highly-functional materials and constructing new science expecting their physical properties, such as the precise forecast of life expectancies and remaining periods, with the essential understanding of the mechanisms.

For this purpose, it is an urgent task to not only analyze the phenomenological macro-characteristics but also to go down to the nanoscale to elucidate the detailed mechanism for the emergence of mechanical properties. In the current situation, however, it is rare for the researchers who cope with the macroscale phenomena, such as those in machine engineering, and those who cope with the nanoscale behaviors, such as those in chemistry or physics, to closely collaborate together to aim at the same target, which hinders the advancement of this research field.

Given the abovementioned, in this research area, we aim at the promotion of the research and development that exceed the space/time scales and the framework of the material types.

2. Principle of invitation project and selection

(1) Basic principle

In this research area, we intend to deepen the research on specific materials and to find a common scientific principle that does not depend on any specific material. For this purpose, our targets include a wide range of fields without being limited to the material type.

However, with any material type, we do not just elucidate the phenomena on the nanoscale but advance the research aiming to link the nanoscale dynamics to the macroscopic mechanical properties and to understand and elucidate the governing factors of macroscopic properties from the dynamic behaviors on the nanoscale. In your proposal, for this purpose, describe the research plans and strategies for linking the nanoscale to macroscale.

(2) Research fields assumed

a. Elucidation of the functional mechanism and governing factors of macroscale mechanical properties from the nanoscale dynamics

- Elucidation of the relationship between the dynamic behaviors of atoms and molecules and macroscale mechanical properties
- Elucidation of governing factors such as the change of nanostructures, dynamics, and chemical reactions influencing mechanical phenomena such as friction, wear, adhesion, joining, peeling, deterioration, and self-healing.
- Findings of academic principles/theory in relation to the improvement of mechanical properties, which has been hitherto understood as the rule of thumb

b. Development of technologies for the measurement, evaluation, and simulation methods of the dynamic behaviors on the nanoscale

- Development of measurement/simulation method to visualize the dynamic behaviors and chemical reactions on the nanoscale
- Development of technologies for the multiscale measurement/simulation method to link the nanoscale to the macroscale under non-equilibrium, dissipative, and/or unsteady state

c. Creation of guidelines for designing the materials to realize new mechanical functions

- Establishment of guidelines for designing the materials that break through the trade-off in mechanical properties
- Establishment of guidelines for designing innovative mechanically functional materials that have never existed before, by using novel technologies such as self-healing and visualization of the governing factor of mechanical properties

In this project, for the development of the guidelines of designing new materials, we recommend the creation of a guideline based on the theoretical backgrounds supported with the new elucidation of the mechanism or supported with a measurement/evaluation/simulation technology, as shown in paragraph "a" or "b" shown above.

(3) Organizations for research implementation

When you make a proposal, organize an optimum research team to realize the proposal in order to accomplish the targets in this research area, such as elucidation of the mechanism for the emergence of mechanical properties of each material type and creation of technologies for

measurement/simulation method of dynamic behavior on nanoscale and of the guidelines for designing innovative mechanically functional materials.

For instance, we can think about the research team in which experiments, analyses, and theories are linked concerning specific materials; the research team that goes beyond the fields of metal and organic materials for the elucidation of a certain mechanical phenomenon; and the research team that conducts the fundamental measurements and/or simulations that are applicable to a wide range of materials and dynamic behaviors. We recommend the proposals that cover beyond fields, such as the establishment of common academic principles that are not limited to specific materials and the interdisciplinary research themes that are not accomplished in any research in the existing specific fields.

(4) Selection policies

a. A novel and original strategy for connecting nanoscale dynamics and macroscale mechanical properties is clearly specified.

b. The “material design guidelines”, which are the output of the research, can be read from the proposal and the goals are clearly identified.

c. High academic or social value when the proposed goal is achieved.

d. Meaningful collaboration between researchers in different fields.

e. A challenging, attractive and innovative proposal. It is not just an extension of the applicant's traditional research.

f. Industrial applicability.

3. Research periods and research funds

The budget for one research project at the beginning is 300 million yen at the maximum (direct expenses).

The research period begins in fiscal year 2021 and ends in fiscal year 2026 (five and a half years or lesser).

Even for the JST-ANR joint proposals, the maximum budget will be allotted to the Japanese side team.

4. Principle of research-area management

In this area, we recommend not only the promotion of the comprehensive understanding on the nanoscale and macroscale concerning specific materials, but also the collaboration among research areas concerning different materials. Furthermore, we advise to be proactive in organizing a community by cooperating not only with those in the same research area but also with those outside your research area, such as "nanoengineering of mechanical functions" in the PRESTO project

implemented under the same strategy target. We expect detailed research for the elucidation of phenomena based on the collaboration among different research areas and the findings of common academic principles concerning different materials.

Furthermore, we want to be proactive in promoting, at the same time as our very fundamental research, the verification of the general-purpose performance of the governing factors and the functional mechanisms of the mechanical properties, and the industrial evaluation of the developed measurement/evaluation methods and the guidelines for designing innovative materials, which are revealed in our research area, in cooperation with some companies. For instance, we are expecting that some breakthrough will be accomplished in a short period such that the innovation of dynamically functional materials may be achieved by converging and applying each achievement and the fundamental knowledge developed in the first half with collaboration among two or more research teams concerning a specific problem of the mechanical properties presented by companies. For this purpose, if it is recognized that the collaboration beyond a research area is effective, the research supervisor may ask you to change the research plans, including the promotion of a joint research and the review of the team organization. In the case of joint Jp-Fr projects, ANR will have to give its agreement for any modification of the Fr scientific tasks and Fr budget distribution beyond the limits stated in the ANR financial regulation. Please refer to the instructions for joint proposal for details.