【Grant-in-Aid for Scientific Research (S)】

Broad Section D

Title of Project : Novel Negative Thermal Expansion Materials for Thermal Expansion Control

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Research Project Number : 19H05625 Researcher Number : 40273510

Keyword : Negative Thermal Expansion, Phase Transition, Local Structure Analysis, Composite Materials, Topology Optimization

【Purpose and Background of the Research】

Thermal expansion arising from anharmonicity of lattice vibrations causes serious problems such as: 1. Deviation of positioning, 2. Deformation, breakage, deterioration of shape accuracy and peeling due to thermal stress. These problems are recognized as a pressing issue in advanced electronic devices such as power semiconductors and three-dimensional integrated circuit devices, and energy and environmental technologies such as thermoelectric conversion and fuel cells, and thermal expansion control is essential for technological innovation. Azuma and Takenaka have developed a new generation of negative thermal expansion materials, which are expected to be able to control the thermal expansion coefficient to an arbitrary value by adding to resins. It is the purpose of this research to establish thermal expansion control technology using giant negative thermal expansion material while developing new materials aiming at industrialization.

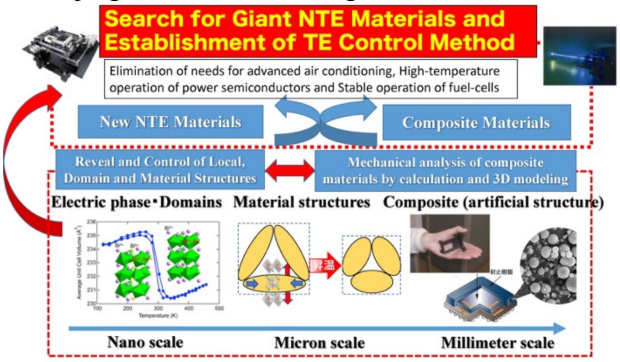

Figure 1 Image of the project

【Research Methods】

Reveal the nanoscale local structure, micron scale domain structure and material structure and structural and mechanical properties of millimeter scale artificial structure fabricated by 3D printing using advanced quantum beams and numerical calculation based on elastic mechanics theory. Furthermore, we will elucidate the phase transition dynamics that is the origin of negative thermal expansion, making full use of first-principles calculations. We will conduct efficient material development by feeding back these results to material design. In addition, a zero thermal expansion composite materials with strong mechanical properties is realized by dispersing the negative expansion material developed in this way into a resin with numerically optimized concentration and arrangement using 3D printing.

【Expected Research Achievements and Scientific Significance】

First, the understanding of the phase transition behavior that influences the negative thermal expansion characteristics will progress, and an efficient material search method can be established. This provides a negative thermal expansion material that can be supplied at a realistic price, followed by a negative thermal expansion of -100 × 10^{-6} / °C over a temperature range of 300°C. In addition, we construct a method to predict the thermal expansion coefficient of a composite material in which a structural material having positive thermal expansion and a negative thermal expansion material are mixed at an arbitrary ratio. Furthermore, by optimizing the placement of the negative thermal expansion material by 3D printing, a structural material with high mechanical strength and an arbitrary coefficient of thermal expansion is realized.

By these, the theory of the negative thermal expansion material and its usage will be constructed, and the problem of the thermal expansion which is socially required is solved, contributing to the further development of precision processing, energy and environmental technology.

【Publications Relevant to the Project】

・K. Takenaka, Y. Okamoto, T. Shinoda, N. Katayama, and Y. Sakai, “Colossal negative thermal expansion in reduced layered ruthenate”, *Nature Commun.*, **8**, 14102/1–7 (2017).

・M. Azuma, W-T Chen, H. Seki, M. Czapsli, S. Olga, K. Oka, M. Mizumaki, T. Watanuki, N. Ishimatsu, N. Kawamura, S. Ishiwata, M. G. Tucker, Y. Shimakawa, and J. P. Attfield, “Colossal negative thermal expansion in $BiNiO_3$ induced by intermetallic charge transfer”, *Nature Commun.*, **2**, 347/1–5 (2011).

【Term of Project】 FY2019-2023

【Budget Allocation】 155,000 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.msl.titech.ac.jp/~azumalab/