Broad Section D

Title of Project : Creation of Innovative Energy Storage Devices Using Atomic Layer Technology

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【Purpose and Background of the Research】

Innovation in energy storage devices is key to addressing mid- and long-term issues in energy and environmental fields, such as energy harvesting from renewable resources and achieving sustainable development goals. Among various energy storage devices, electrostatic capacitors based on dielectric materials have been regarded as one of the most attractive options to develop safe and powerful energy storage devices because of their distinctive features of ultrahigh power densities, ultrafast charge/discharge rates as well as the advantage of not including chemical reactions during cycling, unlike batteries. Dielectric capacitors are thus expected to constitute an ideal, safe, all-solid-state energy storage device. However, the energy densities of dielectric capacitors are generally low, at least 1 ~ 2 orders of magnitude lower than those of batteries and supercapacitors. Continued efforts are being made toward finding dielectric materials with high energy densities.

In this project, we utilize atomic layer technology for exploring innovative energy storage devices. Our approach is to use of 2D nanosheets with high dielectric constants (k). Through multiphase design of dielectric materials/devices from atomic layers to nano-/meso-scale, we aim to develop high-performance energy storage devices based on 2D dielectrics (Fig. 1).

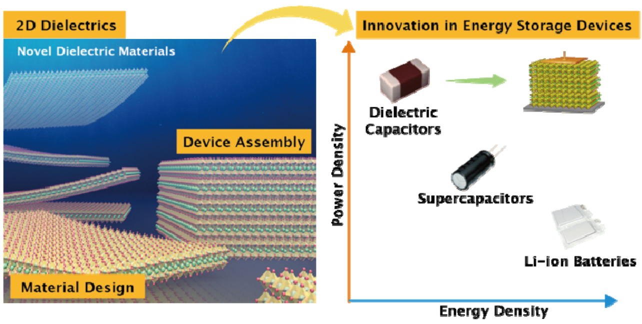

Fig. 1. Overview of our project

【Research Methods】

Conventional dielectric capacitors based on ferroelectric/antiferroelectric materials often yield rather low energy densities because of the inverse correlation between the polarization (P) and breakdown strength (E_b). This trade-off between P and E_b is a well-known dilemma, preventing the development of dielectric capacitors with improved energy densities. 2D dielectrics are principally advantageous for efficiently storing electric energy compared to ferroelectric/antiferroelectric materials; they provide a large capacitance density based on high-k values and molecular thicknesses. Furthermore, the 2D confinement effect induces both an enlarged band gap and an improved breakdown strength, potentially solving the trade-off issue in current materials.

Seeking to investigate these possibilities, we focus on 2D perovskite nanosheets ($Ca_2Na_{m-3}Nb_mO_{3m+1}$; $m = 3 \sim 6$) ($k = 210 \sim 470$) as a model system, and elucidate the mechanism of unique dielectric/ferroelectric properties realized in the ultrathin range (< 10 nm). 2D perovskite nanosheets consist of a few octahedral units (TiO_6, NbO_6 or TaO_6), which make nanosheets an ideal base for high-k dielectric/ferroelectric perovskites with critical thicknesses. Based on these basic knowledge and first-principles-based material design, we aim at not only enhancing dielectric properties ($k > 800$) inherent to the "2D nanostate" but also discovering new dielectric/ferroelectric nanosheets suitable for energy storage devices. Furthermore, we utilize layer-by-layer engineering of 2D nanosheets for developing novel capacitor devices, and realize a remarkable energy density ($U > 10^3$ J/cm^3), which is much higher than that of conventional dielectric/ferroelectric materials and is even comparable to that of Li-ion batteries.

【Expected Research Achievements and Scientific Significance】

2D nanosheets offer unique opportunities for exploring dielectric/ferroelectric properties at the atomic dimension. Through this project, the electronic properties of true 2D systems will be investigated, and novel energy storage devices based on 2D dielectrics will be developed, which will contribute to the generation of novel material technology as well as future scientific and technological innovation of energy storage devices.

【Publications Relevant to the Project】

- Y. Shi, M. Osada *et al.*, "Single droplet assembly for two-dimensional nanosheet tiling", *ACS Nano*, **14**, 15216–15226 (2020).
- B-W. Li, M. Osada *et al.*, "Atomic layer engineering of high-k ferroelectricity in 2D perovskites", *J. Am. Chem. Soc.* **139**, 10868–10874 (2017).
- M. Osada and T. Sasaki, "Two-dimensional dielectric nanosheets: novel nanoelectronics from nanocrystal building blocks", *Adv. Mater.*, **24**, 209–228 (2012).

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