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

Broad Section D

Title of Project： **Paradigm shift in the method for observing non-equilibrium processes in real space: Elucidation of nucleation processes from solution by TEM**

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Research Project Number: 20H05657 Researcher Number：50449542

Keyword：Nucleation, Nanoparticle, Transmission electron microscopy, In-situ observation, Crystal growth

【Purpose and Background of the Research】

Nucleation is a process whereby particles are formed by the agglomeration of atoms or molecules. Because the nucleation process determines the size, crystal structure, number density, and other properties of the resulting particles, an understanding of its mechanism is crucial for the development of materials science. Nevertheless, our understanding of the physical and chemical processes involved in nucleation remains poor. In this project, our objective is not only to achieve an understanding of nucleation process of individual materials, but also to develop a method for determining the physical properties of nanoparticles and elucidating the roles of dehydration, viscosity, and dimer formation in the nucleation process. Consequently, our final objective is to identify the key factors that determine the nucleation route.

【Research Methods】

Our main method is the in-situ transmission electron microscope (TEM) observation of nucleation processes from aqueous solutions. In order to understand the role of the hydrated layer, we have also conducted nucleation experiments from ionic liquid solutions and the gas phase. To observe nucleation from solution samples, we use three techniques (a liquid cell holder (Fig. 1), a solution cell, and a graphene film). These techniques allow us to directly observe the growth rate, shape, assembly, arrangement, and size of the resulting crystals and to identify the phases by electron diffraction patterns. Here, we establish a novel dynamic observation method for non-equilibrium processes using machine learning to visualize the entire nucleation process from solution through precursors to crystal formation by in-situ observation using a TEM.

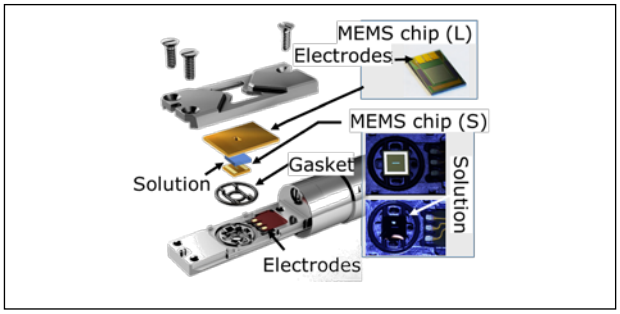

Figure 1 One of three techniques for introducing an aqueous solution into a transmission electron microscope. A liquid cell holder with a heating capability that encloses the solution between two plates with a window. The window is a 30 nm-thick amorphous silicon nitride film, through which electrons can transparent to observe the solution, and the two liquids can be mixed during heating up to 100°C during observation.

【Expected Research Achievements and Scientific Significance】

Because our aim is to identify the key factors that govern the nucleation process and then to construct a nucleation model, our project constitutes groundbreaking fundamental scientific research. After our project, we hope to see a new world in which bottom-up processes for producing nanoparticles and crystals from atoms and molecules can be designed. In addition, we hope to understand the processes involved in the formation of cosmic dust, which consists of nanoparticles with a size of less than 100 nm, and which is abundant in the universe in the gas outflow of dying stars. Furthermore, we will identify conditions that are conducive to the precipitation of metastable phases to facilitate the dissolution of medicines. Thus, the significance and impacts of the results are, potentially, extremely wide-ranging.

【Publications Relevant to the Project】

・ T. Yamazaki, Y. Kimura, P. G. Vekilov, E. Furukawa, M. Shirai, H. Matsumoto, A. E. S. Van Driessche, K. Tsukamoto, Two types of amorphous protein particles facilitate crystal nucleation, Proceedings of the National Academy of Sciences of the United States of America, 114 (2017) 2154-2159.

・ Y. Kimura, K. K. Tanaka, T. Nozawa, S. Takeuchi, Y. Inatomi, Pure iron grains are rare in the universe, Science Advances, 3 (2017) e1601992.

【Term of Project】 FY2020-2024

【Budget Allocation】 154,900 Thousand Yen

【Homepage Address and Other Contact Information】

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