

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

Broad Section C



Title of Project : Dynamical flow control of nanoparticles by machine learning and its application to single molecule identification technologies

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Keywords : Molecular fluid dynamics, Nanoparticles, Single molecule measurement, Machine learning

【Purpose and Background of the Research】

In this project, we aim to comprehensively investigate the flow dynamics of ions, molecules and charged particles in the presence of electromagnetic fields, and to pioneer new research areas. As shown in Figure 1, our approach integrates thermal fluctuations, large deviation principles, thermophoresis, optical pressure, electrophoresis, quantum electronics and machine learning into the field of molecular fluid dynamics. Our practical challenge will be the development of a novel fluidic device with sensing nanogap electrodes for identifying nanoparticles.

【Research Methods】

This project will consist of three different research topics. The first involves the identification of single molecules using a statistical approach to thermal fluctuations. We will define additional dynamics parameters that extend the scope of the fluctuation-dissipation theorem. Novel methods for evaluating and controlling rare events will be developed based on large deviation principles. The second research topic addresses high-speed measurement of the tunneling current between nanogap electrodes, which is a quantum mechanical effect, by sensing nanoparticle flow in a liquid phase based on multiscale electrohydrodynamics (EHD). We intend to establish in situ feedback control of an EHD flow and to design optimized fluidic channels using machine learning. The final research topic

involves manipulation of individual molecules using laser irradiation. The application of optical pressure to drive nanoparticles towards nanogap electrodes will be investigated for the purpose of achieving a higher yield. The thermophoretic force, which can act in a positive or negative direction, and is still not fully understood, will also be utilized. In the second half of the research period, all of the results obtained will be combined in order to develop a micro/nano-fluidic device with embedded nanogap electrodes.

【Expected Research Achievements and Scientific Significance】

By integrating quantum electronics, life sciences, statistical mechanics and information technology into micro/nano fluid engineering, we expect to establish a new academic field called “Moelectro-Fluid Science and Informatics,” and develop new techniques for measuring single molecules utilizing fluidic devices. Such devices can be used for high-speed identification of micro/nano-particles such as pollen allergens, viruses, and DNA molecules.

【Publications Relevant to the Project】

- C. Kawaguchi, T. Noda, M. Tsutsui, M. Taniguchi, S. Kawano, T. Kawai, Electrical Detection of Single Pollen Allergen Particles Using Electrode-Embedded Microchannels, *J. Phys.: Condens. Matter*, 24, 164202, 2012.
- I. Hanasaki, N. Yukimoto, S. Uehara, H. Shintaku, S. Kawano, Linearisation of λ DNA Molecules by Instantaneous Variation of the Trapping Electrode Voltage Inside a Micro-Channel, *J. Phys. D*, 48, 135402, 2015.

【Term of Project】 FY2018-2022

【Budget Allocation】 119,000 Thousand Yen

【Homepage Address and Other Contact Information】

<http://bnf.me.es.osaka-u.ac.jp/>

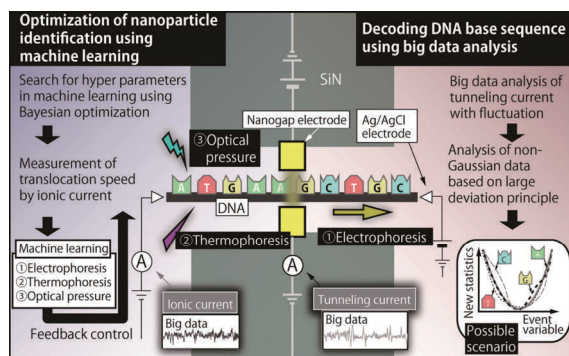


Figure 1 Overview of fluidic device for identifying pollen allergens, viruses, and DNA molecules