[Grant-in-Aid for Scientific Research (S)]

Science and Engineering (Engineering)



Title of Project : The Theory of Microwave-induced Nonequilibrium State and its Application to the Manipulation of Solid/Interfacial Chemical Reactions

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Research Project Number : 17H06156 Researcher Number : 40182985

Research Area : Process/Chemical engineering, Catalyst/Resource chemical process

Keyword : Microwaves, Control of catalytic reactions, Nonequilibrium reaction field, Microwave special

effects

[Purpose and Background of the Research]

Microwaves induce mobile excitation of electrons, ions, molecular structures, and crystal lattices, giving rise to "nonequilibrium states" which cannot be achieved by conventional heating processes. These "non-equilibrium states" occurring at local solid surfaces in a short time lead to not only enhancement of chemical reactions but also selective heating of specific substances (Fig. 1).



Fig. 1, Local thermal non-equilibrium generated under microwave irradiation

We will establish in situ observation methods of short-lived and local non-equilibrium states occurring at surfaces and/or bulk of substances for understanding the theory of specific enhancement of chemical reactions. Our targets are 1) to reveal the mechanism of non-equilibrium states leading to the manipulation of catalytic reactions under microwaves, 2) to reveal specific enhancement and lowering the temperatures in reduction of metal oxides under microwaves leading to a novel smelting technology of metal, 3) to establish a synthetic method of non-equilibrium phase (new compounds, supersaturated solid solutions), 4) creation of new ferroelectric, ferromagnetic, photo-electric, or photo-magnetic materials which are never synthesized by conventional reactions.

[Research Methods]

The joint research group of Wada lab (Tokyo Tech) and Takizawa lab (Tohoku Univ.) will challenge *in situ* observations of "non-equilibrium states" induced by microwaves and apply them to manipulation of chemical reactions.

Target 1: To understand the mechanisms of

non-equilibrium states by *in situ* observation: 1) To design and create *in situ* observation systems, 2) To establish a simulation method of electromagnetic and heat transfer for analyzing heterogeneous temperature distribution, 3) To create a measuring system of absorption capacity of microwaves at microscopic local area.

<u>Target 2 by Tokyo Tech group</u>: To create novel catalytic systems using microwaves.

<u>Target 3 by Tohoku Univ. group:</u> To create novel materials using microwaves.

[Expected Research Achievements and Scientific Significance]

Researches on manipulation of chemical reactions based on thermodynamics and kinetics including catalysts etc. have matured, but we need to challenge chemical activation of stable compounds such as methane and carbon dioxide which requires a novel approach. In addition, we need new materials which can be made using "non-equilibrium state" induced by microwaves. The present study will provide a new generation technology in manipulation of chemical reactions.

[Publications Relevant to the Project]

- T. Ano, F. Kishimoto, R. Sasaki, S. Tsubak<u>i</u>, M. M. Maitani, E. Suzuki, Y. Wada, *In situ* temperature measurements of reaction spaces under microwaves using photoluminescent probes, *Phys. Chem. Chem. Phys.*, 18, 13173-13179, (2016).
- D. Nagao, J. Fukushima, Y. Hayashi and H. Takizawa, Synthesis of homologous compounds $Fe_2O_3(ZnO)_m$ (*m* = 6, 8, 34) by various selective microwave heating conditions, *Ceram. Int.*, 41, 14021-14028, (2015).

Term of Project FY2017-2021

[Budget Allocation] 160,200 Thousand Yen

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