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

Broad Section D

Title of Project : Synthesis procedure of well-defined zeolite and comprehensive understanding of detailed structure

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Keyword : Zeolite, Isomorphous substitution, Precise structure analysis, Synchrotron radiation

【Purpose and Background of the Research】

Zeolites, crystalline microporous materials, are known to exhibit excellent catalytic activity owing to the nanospace originating from the pore structure and the heteroatoms in the zeolite framework. Since they have different pore diameters depending on the framework types, they show a unique shape-selectivity in the catalytic reactions. The catalytic property of the zeolite strongly depends on the type, amount, and location of the heteroatoms introduced into the framework. Although truly important science of zeolites has been regarded as the control and evaluation of the location of the heteroatoms in framework with a microscopic scale and the clarification of the crystallization mechanism, they have not been attained to date. Developments of “well-defined” zeolite and structural analysis method at the “atomic-scale” are indispensable to the solution of these problems and the innovation of zeolite science. In this research, we aim not only to develop the synthesis procedure of well-defined zeolite and innovative structural analysis method based on synchrotron radiation, but also to elucidate the crystallization mechanism and to open a new class of zeolite science.

【Research Methods】

The fundamental knowledge in zeolites from the macroscopic perspective such as crystal structures and functions according to the type of heteroatoms has been accumulated in databases and original papers, and freely available. On the other hand, the characterization of the materials using synchrotron radiation has made remarkable progress in recent years. By combing the fundamental knowledge with newly obtained findings from advanced synchrotron radiation, we will develop a method for identifying the location of the heteroatoms in the zeolite framework at the atomic level. Especially, total/anomalous scattering of X-rays, X-ray absorption spectroscopy, powder X-ray diffraction, and electron density distribution analysis techniques will be applied in order to obtain the structural information of zeolite framework the atomic level.

Simultaneously, we will tackle the synthesis of the “well-defined zeolite” based on "mechanochemical method", "rational choice of cation in synthetic gel", and "design of precursor". These methods can achieve the isomorphous substitution of heteroatoms, and the selective sitting them at the specific sites.

Finally, the thus synthesized well-defined zeolites will be completely characterized by the newly developed structural analysis method, and the crystallization process from an amorphous to a highly crystalline "well-defined" zeolite will be elucidated. Through this research, design and synthesis of zeolite with desired functions, “zeolite informatics”, will be achieved.

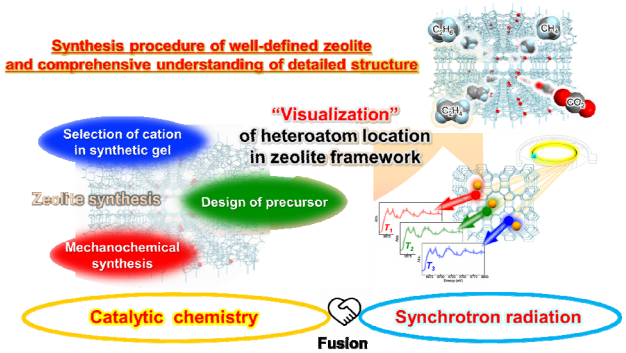

Figure 1 Conception of this research.

【Expected Research Achievements and Scientific Significance】

It is expected to create innovation in zeolite science and a drastic improvement of the industrial catalytic processes, which will contribute to the SDGs. Furthermore, the construction of “zeolite informatics” will lead to the creation of zeolite with a new structure and the expansion of the application. In addition, the establishment of the next-generation synchrotron radiation analysis technique is not limited to zeolite science. It will be applicable to various inorganic and organic materials.

【Publications Relevant to the Project】

- M. Yabushita, A. Muramatsu *et al.*, “Mechanochemical Route for Preparation of MFI-Type Zeolite Containing Highly Dispersed and Small Ce Species and Catalytic Application to Low-Temperature Oxidative Coupling of Methane” *Ind. Eng. Chem. Res.*, **60**, 10101-10111 (2021).
- T. Xiao, M. Yabushita, A. Muramatsu *et al.*, “Organic Structure-Directing Agent-Free Synthesis of Mordenite-Type Zeolites Driven by Al-Rich Amorphous Aluminosilicates” *ACS Omega*, **6**, 5176-5182 (2021).

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