Structuring Knowledge Project in Nanotechnology Materials Program -Construction of a Knowledge Infrastructure for Nano-materials and Devices-

Osamu Kitao[1], Yukio Yamaguchi[1], Eiichi Watanabe[1, 2], Yoshinori Yano[2], Hidenori Yasuda[3], Minoru Miyahara[4], Tadafumi Adschiri[5], Tetsuji Ogawa[1, 2], and Hiroshi Komiyama[1]

[1]Nanomateria Center, 320/322 Engineering Research Institute, School of Engineering, The University of Tokyo, Yayoi 2-11-16, Bunkyo-ku, Tokyo 113-8656, JAPAN, kitao@chemsys.t.u-tokyo.ac.jp,
[2]The Society of Chemical Engineers, JAPAN, [3]Mitsubishi Research Institute,
[4]Kyoto University, [5]Tohoku University

ABSTRACT

The Ministry of Economy, Trade, and Industry, JAPAN has just launched a long-term national program on nanotechnology materials (NMs). This program consists of 8 projects (PJs), and “Structuring Knowledge (SK)” PJ plays an extremely important role among them. Our main focus is on the relationship between process-structure-function for NMs. We here propose our strategy to develop new materials by SK on NMs, as well as completely new simulation technologies. With ontology technology, a “Nanomateria Platform” will give an extremely valuable technological platform for researchers and engineers on NMs, making a major paradigm shift in material industries, and bring us to a new era in material industries.

Keywords: Nanotechnology Materials, Structuring Knowledge, Simulation Technologies, Nanomateria Platform, Ontology

1. INTRODUCTION

Material technology requires a completely new paradigm shift from the trial-and-error approach to well-controlled development, based on fundamental research development and structuring knowledge (SK) on nanotechnology materials (NMs). With worldwide competition on nanotechnology (e.g. national nanotechnology initiative (NNI)), Ministry of Economy, Trade, and Industry, JAPAN (METI) has just launched 8 long-term national projects (PJs) on NMs [1,2]. We here intend to introduce “Structuring Knowledge” PJ [3] (Leader: Prof. Hiroshi Komiyama of Tokyo University; Sub-leader: Prof. Yukio Yamaguchi of Tokyo University; This PJ has been executed by The Society of Chemical Engineers, JAPAN [4]). Our main focus is on the relationship between process-structure-function for NMs. We will construct a database (DB) on a completely new concept based on the distributed and object-oriented information network, “SK on NMs”. To investigate process parameters to make a desired material structure, we will develop a new process simulation package, which studies bulk process mechanism based on multi-scale process simulation technologies with a large scope between nano-meso-macro scales. Moreover, to investigate function on material structure (photo, electronic, and magnetic function etc.), we will develop new simulation technologies that use a realistic force field (FF) completely new simulation technologies.

2. CONCEPT

Materials technology is a fundamental technology for such fields as information processing, environment protection, living environment safety and energy saving. Nanotechnology for materials, as an innovative technology in the 21st century, is expected to revolutionize materials technology. This technology realizes improvement in functions and characteristics of materials as well as creation of new functions through controlling materials structure on a super-fine scale. This PJ will be conducted as a part of the “NMs Program”, the objective of which is to carry out fundamental research and development to systematize obtained research results.

3. MISSION

In this PJ, the purpose is therefore to develop a DB and models from the viewpoint of the process, structure, functional performance and their relations without limiting the scope of materials and to develop a platform that incorporates the above, thereby structuralizing our knowledge of material technology and establish a platform for material development.

4. CONTENTS

Research on the following themes will be carried out in the “SK-PJ in NMs Program”. Figure 1 summarizes the organization of the SK-PJ.

4.1 Establishment of a Knowledge Platform DB

This part constructs the data layer and the bottom of information layer in Figure 1. We focus the target of research on the identification of the architecture of the primary DB by conducting comprehensive extraction of the information items referring to material technology from viewpoint of the processes, structures, and functions involved. The primary DB is to store the body of highly accurate knowledge on material technology by selecting, collecting, ordering and classifying this knowledge from the patents and literature.

to use for development of new materials. SK can change the complex knowledge into valuable information that is easy to use. Moreover the SK indicates what is now known and what is now not known.

Our target is to establish a relationship between process, structure, and function. The native information is induced from the description in the primary DB with the extended make-up language (XML) format. On the other hand, fundamental knowledge on physical chemistry equips information to the multi degrees of freedom in the secondary DB. The proposed multi degrees of freedom are investigated by deducing them to the practical description of the primary DB.

From the mapping from the primary DB to the secondary DB, information on nanotechnology will be mined by visualization, clustering, and estimating model parameters.

Moreover, on the basis of the data of the primary DB, model experiments will be carried out to establish the relationships between structure and function with a view to determining the secondary DB architecture in the light of these experimental results. The data proposed from this PJ, which is implemented under the NMs Program as well as the data of the primary DB, is stored after systematization and classification in the secondary DB. The architecture of the secondary DB will be constantly improved and upgraded in accordance with the availability of model experimental results. This underscores the importance of a flexible architecture that is capable of improvement. Therefore model experiments and each PJ in NMs Program are very important to establish the primary and secondly DBs.

4.2 Development of Modeling

This part constructs the information layer of Figure 1. Based on the information stored in the respective spaces for process, structure and function, this research is designed to develop a modeling engine for calculating and predicting the state of any point in these spaces. A modeling engine is to be developed for simulating the structures formed by the processes. The process structure consistent of the nano-, meso-, and macro-scale. Quantum mechanics and molecular dynamics describe the nano-scale phenomena. Langevin, Brown, Stokes dynamics describe the meso-scale phenomena. The discrete element method and finite element methods describe the macro-scale phenomena. Although each engine can work well for each scale, the connectives are missing between different scales. Therefore we make SK on the process structure, and search public domain codes to make elementary model library. New simulation codes will be developed and added to the library.

Also developed will be a modeling engine for simulating the functions from the structures. Since our interests are especially on photo-, electronic-, magnetic-functions of nano-scale materials, realistic electrostatic FF is essential to study these functions on the nano-scale materials. The FF for a small system can be derived from *ab initio* calculations, and molecular simulation of a small system can be carried out with the use of program code such as Car-Parrinello simulation code. On the other hand, standard molecular simulations can now handle billions of atoms, and the FF should be very reliable at the expense of its lesser complexity to decrease the computational time. Research on the structure-function relationship of nano-scale materials requires alternative methodology, and reliable FF, especially, for the electrostatic interaction part. We are planning to adapt the consistent charge equilibration method [5]. An inferential engine is to be developed for the inference with higher accuracy. For the development and verification of these modeling and inferential engines, development experiments will be conducted for determining the factors governing the nucleation processes, the nucleus coagulation processes, the spinodal decomposition processes, the interface formation processes of NMs and the self-organization control processes.

4.3 Development of a Fundamental Knowledge Platform

This part constructs the knowledge layer of Figure 1. This research develops the platform that provides the environment for easily using the engines developed under research subject 4.2 as well as the DBs developed under research subject 4.1. When necessary, this platform will have the capability of reconstructing the relationship between the DB and the engines and of adding new DBs and new engines. The output image of the knowledge layer is "Nanomateria Platform (NMP)" based on ontology technology.

The meaning of the NMP becomes clear when we consider this SK-PJ in Figure 2. This figure explains the organization of total "NMs Program". This program consists of particle, polymer, glass, metal, coating, and functional materials as the NMs. Material metrology and our SK-PJ coordinate the former six PJs. Within Figure 2, the six former PJs are "Everest attack teams". These teams try to develop new NMs for new functions. Of course, each PJ will perform his systematization for each material, which corresponds to "Base Camp Team" in this figure. On the other hand, the latter two PJs are "Trekking Teams" for the NMs Program. The NMP will provide the knowledge-platform and technology- platform for industries.

This platform is supported by known information on nanotechnology: known algorithm; reliable data from each PJ; known phenomena (e.g. PJ on control of abnormal structure formation on material processing [6]). This knowledge-platform can be of use for decision making on material development to meet some needs for new function, structure, and process. Ontology technology makes the knowledge-platform an extremely valuable technology-platform system for development of new materials. Some ideas in PJ-A may be reused for PJ-B. The SK on NMs makes the transferability very smooth.

5. CONCLUDING REMARKS

METI has just launched a long-term national program on NMs. This program consists of 8 PJs, and "Structuring Knowledge" PJ plays an extremely important role among them. Our main object is to develop the relationship between process-structure-function for NMs. Here we have explained our strategy to develop new materials based on SK on NMs, and completely new simulation technologies. The former knowledge platform consists of the primary and secondary DBs. The development of these DBs makes clusters of complex knowledge on NMs information that is extremely easy to use. The latter new simulation technologies consist of modeling engines to investigate structure based on process information, and function based on structure information. Also developed will be an inferential engine to deduce the structure from the function, organized by a fundamental knowledge platform, NMP. With ontology technology, the knowledge-platform will be an extremely valuable technology-platform system for researchers and engineers on NMs.

We have already submitted the ideas explained here [7], and believe this "Structuring Knowledge" PJ will effect a major paradigm shift in material industries, and bring us to a new era in material industries.

REFERENCES

[1] Y.Yamaguchi and H.Komiyama, "Structuring Knowledge project in Nanotechnology Materials Program Launched in Japan", Journal of Nanoparticle Research, 3, 105 (2001).

[2] New Energy and Industrial Technology Development Organization (NEDO), JAPAN, http:/w w w.nedo.go.jp/kiban/nano/index.html.

[3] NEDO, "First Symposium on Nanotechnology Materials; Towards Structuring Knowledge on Material Technology", 2001/12/12 (in Japanese).

[4] Society of Chemical Engineers, JAPAN, http://www.scej.org/index-e.htm

[5] O.Kitao and T.Ogawa, "Consistent Charge Equilibration (CQEq)", Mol.Phys., submitted.

[6] H.Komiyama, K.Okuyama, M.Matsukata, Y.Egashira, et al., "Control of Abnormal Structure Formation in Materials Processing", www.a-growth.t.u-tokyo.ac.jp/.

[7] H.Komiyama, Y.Yamaguchi, and S.Noda, "Support Procedure on Material Design and the System", JAPAN Patent, submitted.

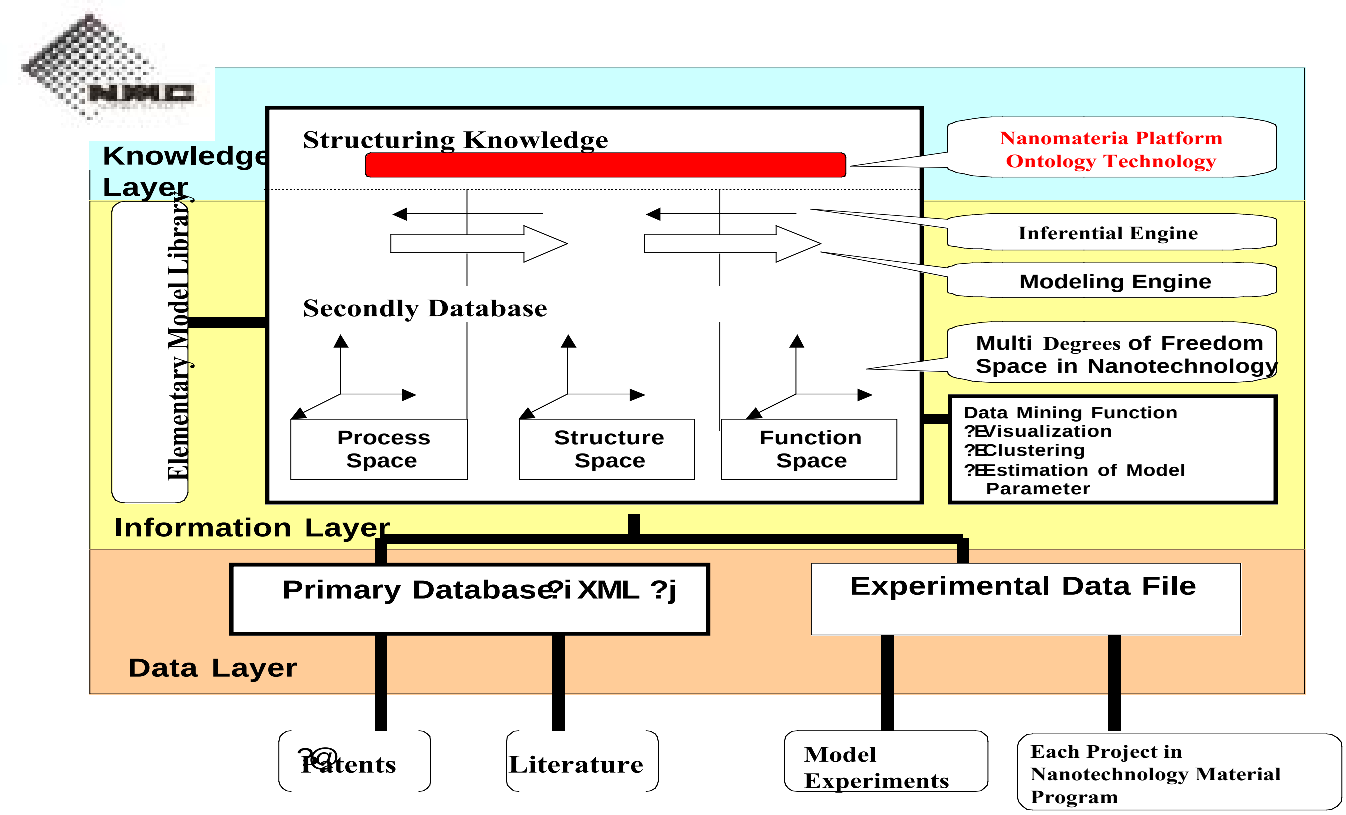

Figure 1. Organization of Structuring Knowledge Project.