

Development of a Design Supporting System for Nano-Materials based on a Framework for Integrated Knowledge of Functioning-Manufacturing Process

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ABSTRACT

In the recent material research, much work aims at realization of “functional material” by changing structure and/or manufacturing process with nanotechnology. However, knowledge about the relationship among function, structure and manufacturing process is not well organized. So, designers have to consider a lot of things at same time. It is very helpful for them to support their design process by a computer system. In this article, we aim to develop a conceptual design supporting system for nano-material. Firstly, we investigate the specifications of such supporting system. And, we outline functionality of the system with some real examples.

KEY WORDS

ontology, nano-material, design support system

1. Introduction

Today, nanotechnology is actively used in different studies conducted in the field of materials science and related disciplines, with the aim of manufacturing materials with specifically enhanced functions or materials having multiple functions. When designers develop such materials, they must consider various requirements simultaneously, such as the functions that the material is to exhibit, the attributes that relate to those functions, and the manufacturing process necessary for producing the material. The number of potential combinations of those items is almost countless, and the items to be considered are very closely related.

In order to develop a computer system that can support the design of such materials, in collaboration with experts in the field of materials science, we have created a model of designers' thinking when they are developing a new material. During this development, we discovered that the functions exhibited by materials and the manufacturing processes are closely related via the attributes in question, and we also learned the issues involved in the simultaneous design of functions and manufacturing processes, as well as in materials design. If we could use a computer system to efficiently assist in such processes before designers actually conduct experiments to verify the combinations and the items that require consideration in the functional design of such materials, it is expected that such assistance will lead to more efficient materials

development and will contribute to the development of new materials.

The aim of our study was to develop a system that can assist designers in such materials design at a conceptual level. To realize such a system, it is essential to systematically store knowledge that relates to the functions of materials and their manufacturing processes and to help designers to design them by making effective use of the stored knowledge. Hence, we have developed a framework for describing knowledge that relates to the functions of materials and their manufacturing processes so that such knowledge can be systematically stored. Based on such a framework, we have developed a knowledge editing system and a design assisting system.

The rest of this paper is organized as follows. In Section 2, we describe the conceptual design covered in our study. In Section 3, we discuss the framework we developed for describing the knowledge of material functions and manufacturing processes. In Section 4, we describe the system that we developed, and in Section 5, we show results of its evaluation and verification. In Section 6, we compare our system with other related studies. Finally, we mention some topics of our future work to conclude this paper.

2. Conceptual design using a function decomposition tree

The aim of our study was to develop a system that aids in the conceptual design of material functions and manufacturing processes using a so-called *functional knowledge-sharing framework* [1]. First, we give an overview of the functional knowledge-sharing framework below.

Generally speaking, a certain function is achieved by realizing a set of sub-functions having a finer grain size. The resulting function achievement hierarchy formed by grouping different grain sizes, which represents the result of functional decomposition in conceptual design [2], is then modeled into a *function decomposition tree*. Within this framework, we describe knowledge about man-made functions in a function decomposition tree (Fig. 1) using the concept of a *functional achievement way* (a way of achieving a particular function), based on the functional ontology that we have developed. Within this framework, it is also possible to describe two or more ways of achieving a single function in an OR-tree (Fig. 2) as

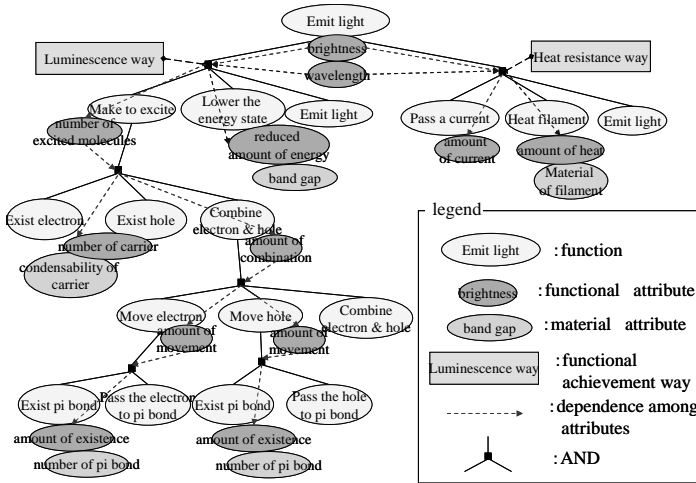


Fig. 4 Function decomposition tree about "emit light"

decomposition tree, as shown in Fig. 5, is referred to as an attribute dependence tree. The attribute dependence tree provides us with better at-a-glance visibility of the dependence among functional attributes than the function decomposition tree.

(3) Functional achievement way information

Functional achievement way information means a description of the properties of each functional achievement way, in terms of its constituent attributes. Here, we describe the properties of a functional achievement way that cannot be expressed in terms of functional attributes and the interdependence of attributes. We can compare properties of one functional achievement way with another through this information. When doing so, it is necessary to describe such functional achievement way information in a more appropriate way. Our framework provides guidelines for describing functional achievement way information, as shown below.

A) Quality of output thing: information about output thing.

A1: Function

-By-product

A2: Manufacturing process

-By-product

B) Quality of process: information of functional or manufacturing process

B1: Function

-Cost of the function

B2: Manufacturing Process

-Cost of the manufacturing process

C: Restriction of object or device in the way

C1: Function

C1-a: Restriction of object (input thing)

C2: Manufacturing process

C2-a: Restriction of object (input thing)

C2-b: Restriction of device in the way

D: Extra information

This summarizes information obtained from interviews we conducted with two materials science researchers in our study.

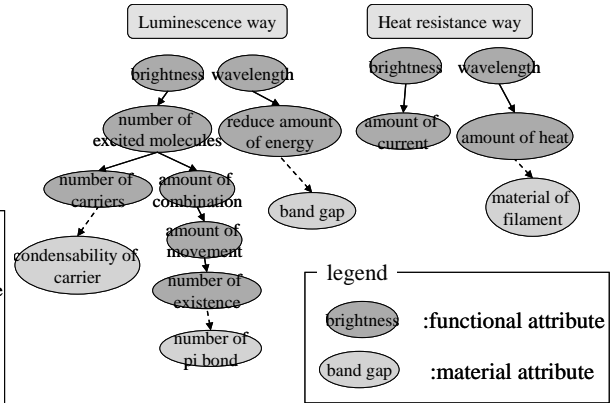


Fig. 5 Attribute dependence tree

3.2 Application to manufacturing processes, and the linkage between functions and manufacturing processes

(1) Extension of functional knowledge-sharing framework toward manufacturing processes

The conventional framework was originally developed for the purpose of systematically describing functional knowledge about man-made articles [1]. However, if we consider a single step in a manufacturing process as an overall function in the function decomposition tree, we can use the same framework to describe the processes of manufacturing products in the same way as for the function decomposition tree. In our study, we call the description of manufacturing processes using the same framework a manufacturing process tree in order to distinguish it from a function decomposition tree. Fig. 6 shows part of a manufacturing process tree for the production of organic EL displays.

In the case of manufacturing processes, we can also consider functional attributes in a similar manner to functions. Since the result of the achieved function in a manufacturing process is a manufactured material, the functional attributes in the manufacturing process indicate the properties that the produced material will have.

(2) Linkage between functions and manufacturing processes

In the function decomposition tree in shown Fig. 3, the function to make something emit light is exhibited by a display as when working as a whole system. The functions located in the bottom tier are directly exhibited by the materials in the electron transfer tier and the light-emission tier etc. On the other hand, the manufacturing process tree in Fig. 5 indicates the process of manufacturing a material that exhibits a function positioned in the bottom tier in the function decomposition tree. This relationship between the functions and the manufacturing processes can also be described in common man-made articles in a similar manner, not only for such novel materials.

If we trace the lines of dependence among functional attributes in the function decomposition tree, we can find out what material we should select and what attributes our selected material should have in order to improve the functions of a product. Furthermore, we can determine the

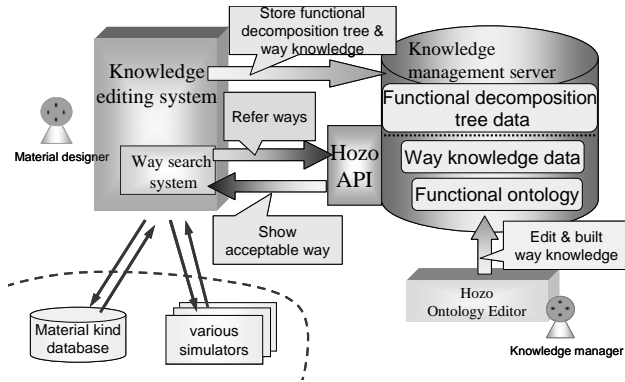


Fig. 7 System structure of Design supporting system for nano-materials

method of manufacturing a material having such attributes by following the path of the dependence among functional attributes of manufacturing processes. In other words, use of the framework described thus far enables us to describe the relationship between the functions in the material decomposition tree and the manufacturing process tree and the relationship among the attributes of both trees, using a consistent framework and keeping continuity.

4. Material Design Supporting System

4.1 System structure

Our system consists of two subsystems: an editing system for integrated knowledge of functions and manufacturing processes (hereafter referred to as the "editing system") and a knowledge management server (Fig. 7).

Materials designers can use the editing system to build a function decomposition tree in order to carry out conceptual design of material functions and manufacturing processes. While doing this, the system allows the designer to operate a *way search screen* to access the accumulated knowledge of functional achievement ways in the knowledge management server, as well as previously built function decomposition trees (results of previous designs), which provides the necessary information to assist in the design process. All function decomposition trees built using the editing system are stored as new design cases in the knowledge management server, to be made available for use in future design work.

The way knowledge accumulated in the knowledge management server is described according to the functional ontology mentioned above and is controlled by a knowledge administrator using an ontology development tool called "Hozo".

4.2 Procedure of material design assistance

The system will provide assistance in the design of new materials, as well as improving the design of existing materials.

To show the procedure used in our system to provide design assistance, as a specific case, we consider here the design of a nano thin film, which is a novel magnetic memory material [3].

(1) Designing the functional structure of a material (building a function decomposition tree)

We design the functional structure by building a function decomposition tree. When doing this, the designer searches for ways that can achieve a required function using the way search screen (Fig. 8). The screen shows a list of ways (1) that can achieve the specified function, selected from the ways accumulated in the knowledge management server; partial functions, functional attributes, and the dependence between attributes (2); and information about each functional achievement way (3).

The screen thus provides the designer with candidate functional achievement ways to review; a group of such ways is shown in section 2 of Fig. 8, which is reflected on the main screen of the editing system. Then, on the main screen, the designer selects a functional achievement way to be used and searches for and adopts ways that can achieve the sub-functions of that functional achievement way. After repeating the above operations, the designer obtains a result, as shown in Fig. 9. The system allows the designer to proceed through the design process by repeating these operations.

During this process, it is important to properly select the required functional achievement ways out of those given by the system. In order to give guidance to the designer in such selection, our system provides three types of information about design cases that used those functional achievement ways in the past, including functional achievement way information showing the dependence of attributes and the properties and restrictions of the particular way, as mentioned in the foregoing section. Using the given information, the materials designer decides the functional achievement ways to be adopted in his or her project; in addition, the designer should add the reason for his or her adoption in the function decomposition tree.

The following section discusses the guidelines given to the designer for those three types of information.

Dependence of attributes

Tracing the dependence of attributes will reveal the attributes of sub-functions that are dependent on the functions to be designed and the functional attributes to be focused on during the manufacturing process (called target attributes). Here, the dependence of attributes varies with the functional achievement ways, and therefore, the functional attributes of sub-functions that are dependent on the target attributes also vary. Thus, one criterion for selecting the functional achievement way to be adopted is whether or not it is easy to change the attributes of those sub-functions. In Fig. 9, for example, a functional attribute *carrier density* of the sub-function control carrier concentration will be dependent on the attribute *number of carriers* if the carrier injection way is adopted, whereas it will be dependent on the attribute *strength of EF* if the *electric field control way* is adopted. Therefore, it is considered better to select the *electric field*

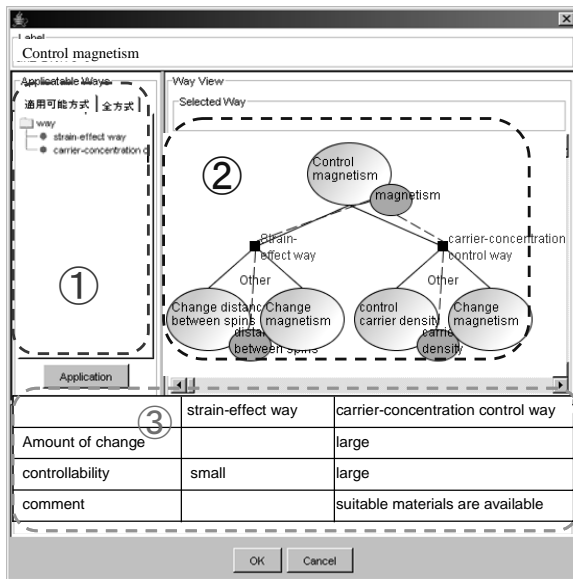


Fig. 8 Way search screen

control way if it is easier to adjust the *strength of EF* than the *number of carriers*.

If it is difficult to make such a decision at this stage, it may be possible to trace the dependence of attributes by further developing the sub-functions of each of the presented functional achievement ways.

Functional achievement way information

The designer selects the functional achievement way to be adopted by comparing the properties presented as functional achievement way information. In 1 of Fig. 9, we can see from the functional achievement way information that, with the *strain-effect way*, *controllability is low*, whereas, with the *carrier-concentration control way*, the *amount of change is large*, *controllability is high*, and *suitable materials are available*.

Past design cases

If the designer checks a presented functional achievement way by asking "in what design cases was it previously studied", he or she can find out the reason why that functional achievement way was adopted (or not) in that case. Such information can be used to determine whether that functional achievement way is applicable to the material currently being designed.

(2) Deciding the attributes of the manufacturing process from the attributes of the material

If the designer traces the dependence of attributes in the built function decomposition tree, he or she can find the attributes of materials that can exhibit a function with the adopted functional achievement way and can continue designing the manufacturing process, focusing on those attributes. In Fig. 10, the designer can trace the dependence of attributes while noting the functional attribute *magnetism* of the top-tier function *control magnetism*, to find that magnetism is dependent on the attributes *number of electrons* and *level of polarization* of

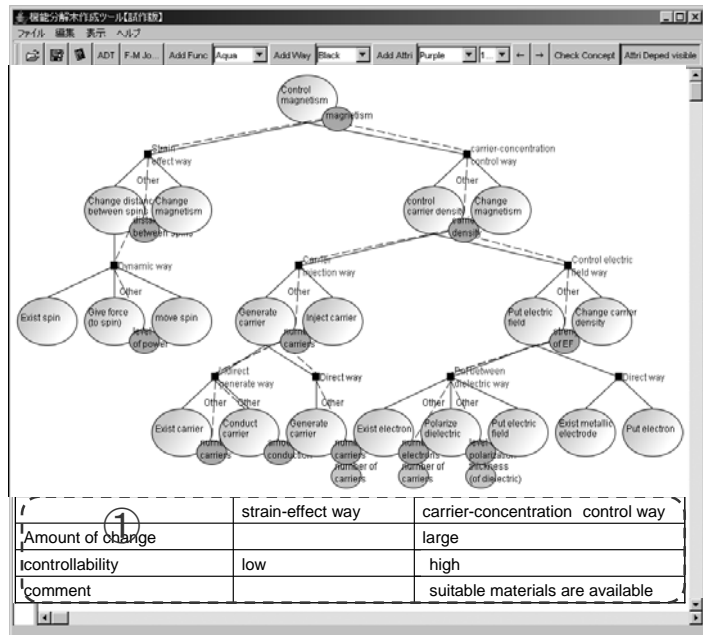


Fig. 9 Example of designing with main screen

the bottom-tier functions, and that these are in turn dependent on the *thickness (of the dielectric)* and the *amount of carriers* of the material that achieves the function.

(3) Designing the material manufacturing process (building a manufacturing process tree)

Noting the attributes of the material selected in (2) above, the designer can build a manufacturing process tree in order to design the manufacturing process for the material. This process should be conducted in a similar way to that described in (1) above.

(4) Improving the design of an existing material

If the designer wants to improve the value of a target attribute, for example, or she may carry out design to improve the material functions and/or manufacturing process, if necessary. There are two methods to do this:

- Recursively trace the functional attributes of sub-functions that are dependent on the target attribute, find some attributes that are easily changeable, and make adjustments.
- Noticing that the dependence of attributes varies with the functional achievement way, change the selected functional achievement way to an alternative one in order to improve the value of the target attribute.

Since our system manages the dependence between functions and manufacturing processes, it allows the designer to consider the attributes of functions and manufacturing processes in an integrated manner.

5. Assessment

5.1 Verification of descriptive capability

In order to verify the effectiveness of the framework for describing knowledge about material functions and manufacturing processes which the system provides, we attempted to describe specific cases of actual materials

Table 1 Data for the two general function decomposition trees built by subjects

Subject		Prior Knowledge	Correct or Wrong	Number of Indicated Paths	Design Duration (min.)	Number of Adopted Ways	Criteria for Adopting the Function Achievement Way				
							Way Information	Dependence	Way in a Lower Tier	Name of Way	Prior Knowledge
Material Researcher	A	1(1,2,3)	OK-1	2	9	5	0	0	1	2	2
	B	1(1,2,3)	OK-1	18	18	6	5	0	2	0	3
	C	2(1,2,4)	OK-1	8	14.5	4	0	0	2	0	2
Student of General on Material Science	D	3(4)	OK-1	22	15	6	1	0	2	2	0
	E	3(4)	NG	23	22.5	6	4	2	0	0	0
	F	4(5)	NG	26	22.5	8	5	0	1	2	0
	G	4(5)	OK-2	17	27.67	6	3	0	1	2	2
	H	4(5)	OK-1	14	22	6	4	1	1	0	0

Correct or Wrong: Agreement with a correct function decomposition tree prepared based on the experts' design, indicated by the following symbols: OK-1: Subject's best design agrees with the correct answer; OK-2: Subject's second best design agrees with the correct answer; and NG: no agreement.

Number of indicated paths: The number of combinations of selectable functional achievement ways (in a section of an OR-tree) in the general function decomposition trees submitted by subjects. This can be considered the number of combinations that were evaluated during the design process.

Design duration: The time required to complete the two designs.

Number of adopted functional achievement ways: The number of functional achievement ways decided to be adopted from multiple candidates in the two function decomposition trees built by the subjects.

Criteria for adopting the functional achievement way: The criteria used by the subjects when adopting the functional achievement way. The reasons given by the subjects for adoption of the functional achievement way were analyzed and classified into the following five categories:

- **Functional achievement way information:** The subject referred to the information presented by the system in the form of functional achievement way information.
- **Dependence:** The subject referred to the interdependence of attributes.
- **Name of functional achievement way:** The reason may have been inferred from the name of the functional achievement way.
- **Functional achievement ways in a lower tier:** The subject referred to functional achievement ways in a lower tier.
- **Prior knowledge:** When none of the above applies.

If two or more types of information are given as the reason for adoption and each type of information is classified into separate adoption criteria, then all criteria should be counted.

(3) Analysis

Analysis of design results

Before analyzing the design results, all subjects were divided into two groups: Group 1 included those subjects who had directly received, from an expert, some explanation about the magnetic material to be designed, and Group 2 consisted of the remaining subjects. The results were sorted and put in order according to group; they are shown in Table 2. Each item is described below:

Correct answer ratio: The percentage of subjects for which either of the two answers agreed with the correct answer (indicated by OK and NG in the Correct/Wrong column in Table 1).

Average number of indicated paths: The average number of indicated paths in Table 1.

Average design duration: The average duration of the design in Table 1.

Percentage of adoption criteria: The ratio of (total number of adoption criteria) / (total number of adopted functional achievement ways) in Table 1.

First, for all members of Group 1, their Best answers agreed with the correct answer, and for Group 2, 60% of subjects produced correct answers, including their Second best answers. This indicates that, without having prior knowledge of the design-target material, the subjects could design a functional structure according to the given requirements if they have common knowledge about the material.

Second, looking at the proportion of criteria for adopting the functional achievement way, almost half of the members of Group 1 selected "Prior knowledge", while a little more than 50% of Group 2 selected "Functional achievement way information" as the adoption criteria. This indicates that the guidelines for selecting the functional achievement way provided by our system could help beginners who have little prior knowledge about the conceptual design of material functions.

Out of all 16 design results, we analyzed 10 functional structures that failed to agree with the correct answer set in collaboration with the experts. Six results met the requirements, proving that they were feasible, and we found that we could consider them correct answers

Table 2 Sorted and put results in order according to groups

Group	Correct Answer Ratio	Average Number of Indicated Paths	Average design duration (min)	Percentage of Adoption Criteria				
				Way Information	Dependence	Way in a Lower Tier	Name of Way	Prior Knowledge
1	100% (3/3)	9.33	13.83	33%(5/15)	0%(0/15)	33%(5/15)	13%(2/15)	46.7%(7/15)
2	60% (3/5)	20.4	21.93	53.1%(17/32)	9.3%(3/32)	15.6%(5/32)	18.8%(6/32)	6.25%(2/32)

Table 3 Result of answers of questionnaire

Subject	Evaluation	Contribution to Material Design			
		Function decomposition tree	Function Attribute	Dependence of Attributes	Way Information
1	A	5	4	5	3
	B	4	4	5	5
	C	3	5	4	5
	Z	5	4	4	5

although they did not agree with the set correct answer.

Furthermore, one of them indicated a novel functional structure, which even the experts had not thought of. The possibility of realizing this idea is now under discussion by experts. This suggests that the system has the potential to contribute to the creation of fresh ideas.

Results of answers to questionnaire

After the experiment, a questionnaire on the effectiveness of the system was circulated to researchers in materials science and related fields, including the test subjects. The collected answers are summarized in Table 3. The items in the questionnaire were as follows:

(1) Evaluation: "Do you want to use this system for your own research in the future if sufficient functional achievement ways are stored in the system?"

(2) Contribution to materials design: "Do you think the elements of the description framework used in this system (i.e., the function decomposition tree, functional attributes, dependence of attributes, and functional achievement way information) are helpful to design materials' functions?"

Answers to both questions were requested to be given on a five-point scale (5 for best), and subjects were asked to freely describe the reasons for their evaluation. For example, we received the following answer to Question (1): "Seeing the function decomposition tree enabled me to understand the basics of the field of study, which is outside my major". This convinces us that the system has the possibility of contributing to materials design. Another answer opined that it would be more effective if there were sufficient accumulation of functional achievement way data, saying, "I think the system would be more attractive if the number of choices of functional achievement ways was increased and made more specific". In Question (2), all the respondents gave five points to "Dependence of attributes". As for the percentage of adoption criteria in Table 2, none of the Group 1 subjects chose "Dependence of attributes". We interpreted this as meaning that they might have thought it would be helpful in the design of other materials' functions because "dependence of attributes" was not used by chance for the design of the material functions covered by this experiment.

6. Comparison with related research

Mase et al. have been developing a machine design assisting system based on a so-called thought expansion plan [3]. Their system lets designers describe a thought expansion plan in order to sort out the designer's thoughts, and presents annotated documents and CAD data to the designer using a thesaurus, thus assisting designers in

creating ideas, coming up with solutions to constraints arising during the design process, and inheriting knowledge of the design method. Their system and ours have different approaches to design assistance. In the system of Mase et al., technical terms and other thesauri serve as the basis for presenting knowledge to designers; however, this approach has the problem that designers in a slightly different discipline cannot understand the terms because technical terms vary from field to field. On the other hand, our system presents knowledge that is independent of the discipline; it presents functional achievement way knowledge and additional information based on a functional ontology. Consequently, knowledge coming from different disciplines can be understood by designers, possibly assisting in the creation of original ideas, independent of the discipline.

In addition, there is TechOptimizer[4], a software package for idea assistance. This software works on the TRIZ theory; if we specify the target functions and the method to achieve them, the software will display a list of cases that use the method and an explanation of the inventive principle in those cases. However, the inventive principle is often highly abstract, and the tasks of making an exact model of the design objective and applying the inventive principle to the model are left entirely to the designer. Furthermore, the TRIZ theory presents an inventive principle mainly to overcome a trade-off, whereas our system performs design assistance from the designer's viewpoint, centered on functions, and is not intended to solve the trade-off.

Stone et al. are pursuing research aimed at conceptual design using a standard function vocabulary, just like our system [5]. Using a standard function vocabulary called Functional Basis, their system describes a functional model of existing products, and separately from that functional model, it builds a matrix of the linkage between functions and components and the linkage between components from a prepared repository; then, based on this matrix, its algorithm automatically generates variations of conceptual designs. This algorithm, however, can cover only designs by analogy from existing articles, and Stone et al. themselves point out that it cannot design a new item. In contrast, our results indicate that our system has the possibility of designing new materials through the combination of existing knowledge.

7. Conclusion

In this paper, we have described the development of a system that assists materials designers at a conceptual level. First, we discussed a model of the thinking of experts in materials development when they perform conceptual design of materials, based on the framework of advanced research that has been conducted in mechanics and related fields. Then, based on the above, we developed an integrated knowledge framework for functions and manufacturing processes that systematically describes knowledge related to material functions and manufacturing processes. On the basis of this framework,

we then developed a design assisting system. We verified the descriptive capability of our system and the effectiveness of its design assisting functions in collaboration with experts in materials science, taking the material functions and manufacturing processes that they actually developed as specific cases. Through these processes, the experts suggested that this system has the possibility of contributing to materials design.

In the future, we will attempt to extend the functional achievement way knowledge and to enrich the functions of this system while building material decomposition trees and manufacturing process trees through interviews with experts.

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