Establishment of a database on thermophysical properties of melts

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Abstract

We tried to develop a database on thermophysical properties of melts for making smooth progress in the diffusion project, which is one of the research projects in NASDA. In this year, followings were performed.

- Establishment of the concept of the database.
- Organization of the database based on this concept.
- Confirmation of the functions of the data base.

1. Intoroduction

NASDA has several research projects. The project "Modeling and Precise Experiments of Diffusion Phenomena in Melts under Microgravity" is one of such research projects in NASDA. In this project, we study diffusion phenomena in melts by means of various tools, such as theories, simulations, and experiments in order to realize the precise measurements of diffusion and to establish the model of diffusion in melts. The project has incorporated scientists from various research fields, such as liquid theories, molecular dynamics simulation, neutron scattering, and development of experimental setup including the computer fluid dynamics. Therefore, our project is an interdisciplinary project.

For making smooth and efficient progress in this interdisciplinary project, it is very important to achieve a consensus among the team members of this project about the aim, the schedule, the method of approach, and the results in this project. Moreover, it is necessary to exchange opinions and views based on the communal information each other frequently and quickly. At present, electronic information technologies are advancing rapidly. Almost all the researchers use the e-mail and internet communications by their own personal computers. Therefore, it is far easy to exchange views and opinions each other by these electronic communication tools. It is not always necessary to gather all members at one place for the meeting.

Therefore, what is important is to have the communal information and to construct the network for the exchange of views and opinions among team members. For this reason, we try to collect the communal information to team members, such as the thermophysical properties, experimental results etc., and to organize these data as the database for the study of our project.

2. Preconditions for developing the database

At first, it is better to determine the precondition for establishing the database because the required function of the database depends on the purpose of users. From this point of view, we determined the following three preconditions.

1) <u>As a first step, the present database is open only to team members of the diffusion project.</u>

It is very helpful to collect and open the thermophysical data of melts and other related

data to the diffusion in melts obtained in this project. And in this database, we try to include raw data about experiments or simulations during the study. But almost all those data are the intellectual properties for the scientists before they report to the journal so on.

Therefore, as a first step, the present database is open only to team members of the diffusion project

2) The data is stored in the database in the form of the HTML file or PDF file.

Each researcher is using a different OS system, such as Windows, Macintosh, etc. However, it is possible to see the HTML file and the PDF file by almost all computer machines that include WWW browser and/or Acrobat Reader, which is distributed by Adobe.

3) The content of database is distributed to team members of diffusion project by using CD-ROM until the content of the database is abundant.

Nothing to say, it is convenient and appropriate to deliver the data by the internet. But we have to consider the problem of the administration and the maintenance of servers and the security of data.

3. Establishment of database concept

At first, for developing the database, we establish its concept. Fig.1 shows the structure of the database in our project. It consists of two main parts, which is Conference part with two subparts ant Data part with four subparts. We set up a password on front-page for the utilization of this database only by team members of this project. The followings are the contents of each subpart. In this database, there are same data among subparts, so we link them each other and we can gain access to them from various parts.

(1) Front-Page

Based on the precondition, this database is open only to team members in this project. Therefore, in the front-page, the password must be inserted in order to restrict the utilization of this database only to team members.

(2) Schedule

In this part, the conference and meeting schedules of the project will be shown.

(3)Conference and Meeting Database

The reports of members and minutes in each conference or meeting are inputted into this part as the documents of progress of the project.

(4) Experimental Database

"Experimental Database" part includes summaries of papers or reports of the microgravity experiments conducted in Japan and in other countries. As the reference data for the performance of experiments or numerical simulations, we collect the original data and the analyzed final form of data of these microgravity experiments as possible as we can. This is helpful for team members of the present project to check the results each other and to possess a communal information. Not to mention, by password the access to these data is restricted only to team members. In addition, this part includes experiments and simulations which are not directly related to the microgravity but are important for the study of the diffusion in melts.

(5) Simulation Database

"Simulation Database" part includes simulations, such as molecular dynamics simulations, and the others related quantities, such as interatomic potentials and physical properties required for simulations.

(6) Physical Property Database

"Physical Property Database" part includes thermophysical properties required for the advance of the diffusion project, such as, density, viscosity, surface tension, thermal conductivity, etc. Particularly the highest priority is given to thermophysical properties of the target materials for the diffusion project. Thermophysical properties of other materials related to the diffusion study are also being inputted with the progress of the diffusion project.

(7) Paper Database

Outline of the papers related to the diffusion study are inputted. This part consists of following five parts, 1) Physical Properties, 2) Molecular Dynamics Simulation, 3) Experimental Equipment, 4) Reports, and 5) The others. But these classifications will be changed in the progress of the project by taking into account of the opinions of team members.

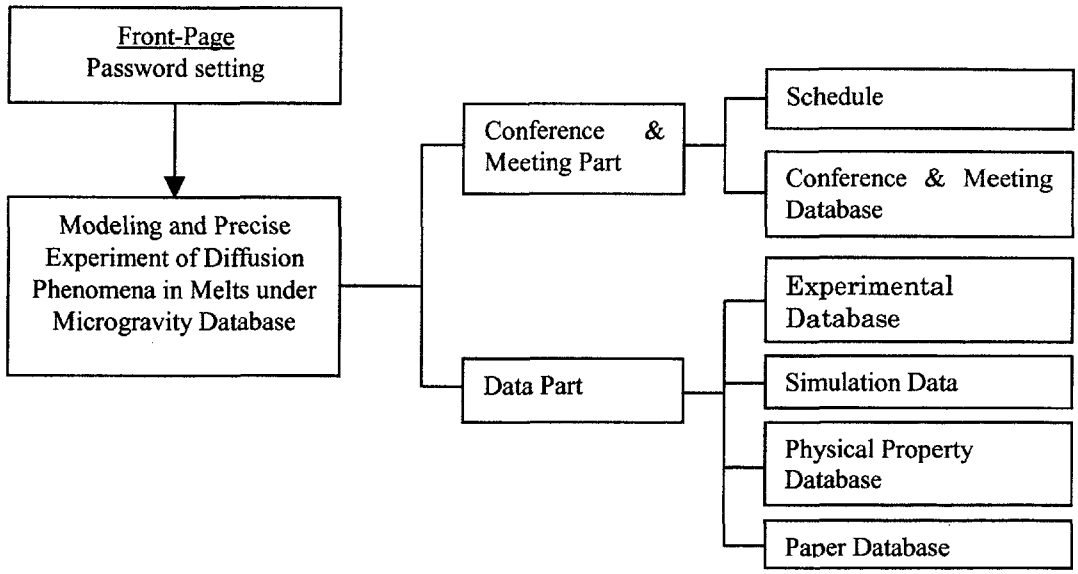

Fig.1 Database Structure

4. Results

Based on the database structure shown in Fig.1, we developed the database, confirmed the validity of its function and the hyper-link between subparts. Finally it was inputted on CD-ROM and distributed to team members at each conference or meeting. Tab.1 shows a list of data inputted into the present database. At the present trial period, we input each data as a picture data. Therefore it is impossible to retrieval (or search) the data in the present database by key word. This demerit is partially compensated by the link among subparts of the present database, by which we can approach same data from different subparts.

5. Conclusions and Future plans

This trial database is developed as one part of the activity of NASDA diffusion project under precondition that only team members of the diffusion project can enter into it. However, we think

that it is valuable and useful to open our database to the public. It provides a good chance to present the results and the activities of our diffusion projects, which should be widely utilized. From the viewpoint of release to the public of the present database, there are some problems, such as the copy light, the absence of the search function by key word, and so on. Therefore, next year we discuss how to improve our database to open it to the public. On the other hand, it is important to have communal data, which include raw data about experiments or simulations, among team members. For this purpose, we also make this database to be much abundant in data related to the diffusion in melts.

Tab1 List of the data inputted to database

Item	Contents
1. Conference and Meeting	Minutes(Documents) and Materials of the first and second meeting in 1999
2. Experimental Database	
Experimental data of Pro.Itami	Data before analyzing
FMPT	Outline of Dr. Dan's report
TR-1A#4 (PbSnTe)	Outline of Dr.Uchida's report
TR-1A#5 (Ge)	Outline of Pro.Itami's report and Dr.Yoda's report
TR-1A#6 (Li) *	Outline of Pro. Itami's report
MSL1	・Outline of the results of MSL-1 ・Outline of Technical Report of NASDA ・Outline of Special Issue : MSL-1(1)
SL-1	・Some results of SL-1
SL-D1、D2	・Some results of SL-D1, D2
EURECA	・Some results of EURECA
TEXUS	・Some results of TEXUS
3. Simulation Database	
MD Simulation	Simulation code developed in 1998 is inputted.
Potential Model	Refer to "Papers Database"
Physical Properties	Structure factor, Density, Surface tension (Refer to "Physical Properties Database")
4. Physical Properties Database	
Ge	Density、Viscosity、Surface tension、Volume expansion coefficient、Thermal conductivity、Specific heat
Li	Density、Surface tension、Viscosity
Sn	Viscosity、Surface tension、Volume expansion coefficient、Thermal conductivity、Specific heat
Si	Density、Viscosity、Surface tension、Volume expansion coefficient、Thermal conductivity、Specific heat
Sb	Density、Surface tension、Viscosity
Pb	Density、Surface tension、Viscosity
In	Density、Surface tension、Viscosity、Thermal conductivity、Specific heat
PbSnTe	Dr Uchida's report
GaAs	Density、Viscosity、Surface tension、Volume expansion coefficient、Thermal conductivity、Specific heat
GaSb	Density、Viscosity、Volume expansion coefficient、Thermal conductivity、Specific heat
Cu-Ag	Pro. Yamamura's report presented to NASDA
Others	・Some data of thermodynamic and transport properties of Alkali Metals ・The Structure of Liquid Metals and Alloys ・Some data of Mo and Ta