# Function Sharing and Systematic Collaboration between a Networking Database System and Printed Media on Thermophysical Properties Data†

**Tetsuya Baba,*,‡ Yuichiro Yamashita,‡ and Akira Nagashima§**

National Metrology Institute of Japan, AIST Tsukuba Central 3, 1-1-1, Umezono, Tsukuba, Ibaraki 305-8563, Japan, and Keio University, 3-14-1 Hiyoshi Kohoku-ku, Yokohama, Kanagawa 223-8522, Japan

To improve the performance of devices, components, and systems where the control of heat and fluid flow are necessary, the quality and reliability of the thermophysical property data are of primary importance. Recently, the present authors have worked for both printed media, a new handbook, on thermophysical properties and a networking database system. From this experience, the authors realized different advantages of both tools and started to explore function sharing and collaboration of these tools. The present paper describes the conceptual trials although the study is in its early stage. The *Thermophysical Properties Handbook* edited by the Japan Society of Thermophysical Properties (JSTP) first published in 1990 was revised in 2008. It stores thermophysical properties of not only basic materials such as elements, basic chemicals, and compounds in fluid and solid phases but also materials for variety of application fields such as energy, chemical engineering, metallurgy, electronics, air conditioning, and so on. Although the handbook is published as the form of a printed book at present, JSTP has been digitalizing the thermophysical property data of the handbook and supplying them as content in a database. On this basis, JSTP and the National Institute of Advanced Industrial Science and Technology (AIST) agreed to develop a network database system for thermophysical property data. It was realized that disadvantages of a computerized database exist against obvious advantages such as quick revising/upgrading, easy interpolation, and converting in graphical expressions. Both the printed media and the networking database system have different functions and advantages. The intention of the present paper is to explore more beneficial means to access reliable thermophysical property data for users, especially in industry.

## 1. Introduction

To improve the performance of industrial systems, chemical plants, or electronic devices, where the control of heat or fluid behavior is necessary, the availability and reliability of thermophysical property data are of primary importance. In earlier times, data books were used as the source of the information, and in more recent times, a computerized database has been overwhelmingly used as the more convenient tool.

Thermophysical property data can be retrieved from the data books which cover a wide variety of physical and chemical data such as the *Landolt−Börnstein Data Series*[1] and *The CRC Handbook of Chemistry and Physics*.[2] Since they have been compiled from scientific data over general physics and chemistry, they are not focused to cover thermophysical property data for industry comprehensively. Now, Springer provides search function enabling users to find specific Landolt−Börnstein documents at the website.

The *TPRC Data Series*[3] are still useful at present, although they are mainly based on experimental results of thermophysical property measurements from more than 40 years ago. The Center for Information and Numerical Data Analysis and Synthesis (CINDAS, West Lafayette, U.S.A.) at Purdue University has developed a web-based database of thermophysical property data compiled from the *TPRC Data Series*.[4]

The Institute for Nuclear Technology and Energy Systems (IKE) group for thermophysical properties at the Stuttgart University has developed a database named THERSYST for thermophysical properties on the basis of data measured in their laboratories and from literature.[5] THERSYST has been inherited by Evitherm, European Virtual Institute for Thermal Metrology.[6]

To evaluate critically the available experimental information on the properties of pure fluids and to produce internationally acceptable tables of these properties for use in science and industry, the IUPAC Project for Thermodynamic Tables was initiated in 1965 under the auspices of IUPAC Commission 1.2.[7] The project centre was founded at Imperial College in London.[8] The centre has published 12 volumes in the series, *International Thermodynamic Tables of the Fluid State*.[9] The activity of Commission I.2 on thermodynamic properties was succeeded by the International Association of Chemical Thermodynamics (IACT).

The subcommittee on transport properties of Commission I.2 was also founded to make critical evaluations and to propose standards of transport properties of gases and liquids.[9] In 2001, following a reorganization of IUPAC, the subcommittee's existence was terminated, and the activity was succeeded by the International Association for Transport Properties (IATP).

The *Journal of Physical and Chemical Reference Data* is published by the American Institute of Physics (AIP) for the National Institute of Standards and Technology (NIST) to provide critically evaluated physical and chemical property data.[10]

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* Corresponding author. E-mail: t.baba@aist.go.jp.
‡ National Metrology Institute of Japan. Tel.: 81-29-861-4053. Fax: 81-29-861-4236.
§ Professor Emeritus, Keio University. E-mail: nagasima@sd.keio.ac.jp.

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The *Journal of Chemical and Engineering Data* is published by American Chemical Society to provide experimental data and the evaluation and prediction of property values of physical, thermodynamic, and transport properties of well-defined materials.[11]

The Thermodynamics Research Center (TRC) of the Thermophysical Properties Division at the NIST in Boulder, Colorado, U.S.A., specializes in the collection, evaluation, and correlation of thermophysical, thermochemical, and transport property data and has been engaged in the production of a large number of the periodical compilations and databases for recommended data of both pure materials and mixtures.[12]

Two series of periodicals containing evaluated data for pure compounds (*TRC Tables - Hydrocarbons* and *TRC Tables - Non-Hydrocarbons*) have been published by TRC for many years. Recently, a web version of the TRC Tables, called Web Thermo Tables (WTT), has been developed.

The importance of standard formats of thermophysical and thermochemical property data was accelerated by the progress of information technology resulting in the wide use of PCs (personal computers) and the Internet. *ThermoML: XML-Based Standard for Data Storage and Exchange* as a standard format for data storage and exchange was developed by TRC within IUPAC Project (2002-055-3-024): XML-Based IUPAC Standard for Experimentally and Critically Evaluated Thermodynamic Property Data Storage and Capture.[13,14]

Historically, TRC, then with Texas A&M University, developed the first prototype of such a standard called COSTAT (COdata STAndard Thermodynamics) from 1985 to 1987, and ThermoML at TRC is a result of further improvement of the basic principles defined in COSTAT.

TRC cooperates with five journals including the *Journal of Physical and Chemical Reference Data* to accumulate data in the format of ThermoML.[15]

The major databases mentioned above are operated by data centers which are responsible for all management, including maintenance of the database server, registration and updating of data, and improvement of the database management system.

On the contrary, the AIST has proposed a network database system for thermophysical property data under which a number of organizations collaborate to operate the database by registering and updating thermophysical property data of specific substances/materials or application fields in which they have been engaged.[16] This database has been developed in close collaboration with the JSTP which is engaged in revision of the *Thermophysical Properties Handbook*.[17]

The present authors have worked for both printed media, a new handbook, on thermophysical properties[18] and a networking database system. From this experience, the authors realized different advantages of both tools and started to explore function sharing and collaboration of these tools. The present paper describes the conceptual trials, although the study is in its early stage.[19]

In the case of a data book, a typical printed medium, data contents are normally listed in a systematic and well-designed style. The obvious advantage is not only an easy, bird's-eye view of data but also a systematic ordering or structural relation of the substances/materials. Listed data in the established data book can be considered reasonably reliable since they are often pre-examined or pre-evaluated to some extent. The editorial committee is responsible for guaranteeing that listed data are to be checked or at least read by more than one author. Data are printed and therefore cannot be revised easily. This is disadvantage, of course. However, in the viewpoint of information security, this is an advantage. So, the most important advantage of printed media is, generally speaking, first-hand reliability.

Of course, a networking database also can provide various ways to check reliability as mentioned later. However, it has the possibility of less-confirmable reliability due to very easy reconstruction and the possibility of danger in security due to network penetration. Recently, one of the authors, Nagashima, at Keio University, pointed out the danger of "recovery of once-killed data". In the past, some data were criticized as wrong by groups of experts and excluded from recommended list. However, because of dramatic development of Internet searching technology, "once-killed data" repeatedly appear on the surface and are used as one component of averaging.

Systematically arranged data in a data book often can provide some kind of milestone instruction to users who are an expert in another field but a newcomer in that particular field. This also can, in broader use, provide tools for the education of young students.

Considering these advantages, the new edition of *Thermophysical Properties Handbook* was published in 2008 as explained in the next section.[18]

On the other hand, advantages of a computerized database are well-realized such as fast, easy, and wide access to pinpoint data. It is easy to upgrade or revise the database to the new version. There are many possibilities to explore new and original uses for data such as the inverse search of substance/material from data, and so on. It is possible to start database−user and user−user collaborations. Two of the present authors, Baba and Yamashita, at AIST have worked to establish the networking database system called "Thermophysical Property Data System, TPDS" as explained in Chapter 3.[16] The network is the product of collaborations among many thermophysical-property researchers, the JSTP, and AIST.

Now, as the next stage, the present authors intend to explore function sharing and collaboration among the printed media, the new handbook, and the networking database system. Each of the two tools has different functions and advantages. The intention of the present paper is to provide more beneficial means to access reliable thermophysical property data for users, especially in industry. Some results are appearing, although the study is still in its early stage.

## 2. New Edition of the *Thermophysical Property Handbook*

***2.1. Thermophysical Properties Handbook.*** The first edition of the *Thermophysical Property Handbook* edited by the JSTP was published in 1990 to supply comprehensive and systematic information of thermophysical properties to many scientists and engineers who use and/or produce thermophysical property data.[20] Now, it has been revised corresponding to recent progress of science and technology.

Since thermophysical properties are basic and common information for the extensive field of science and technology, a collaboration of researchers over a variety of scientific and technological communities, such as thermal engineering, chemical engineering, materials production, electronics, geology, domestic science, life science, and environmental technology, has been necessary to compile the handbook.

For example, to improve productivity of industry, numerical simulation is one indispensable tool to design new products and to specify optimum conditions of manufacturing process replacing experience, skill, or trial-and-error approach. Simulation has been introduced to mature industries such as injection molding

or casting as well as an advanced industry such as the thermal design of an electronics devices, production of semiconductor crystals, and phase change control of optical memory devices. Quantitative simulation must be based on reliable thermophysical property data of the materials constituting the system or device.[21–23] Comprehensive thermophysical property data are stored in the handbook with common definition, terminology, and description. The handbook also provides broader systematic information on how to search, access, measure, and evaluate thermophysical properties.

***2.2. Some Specific Features of the Handbook.*** The new edition of the *Thermophysical Property Handbook* is designed for users in broad scientific and technical fields to search thermophysical property data of not only their own field but also other fields efficiently.

The handbook consists of four parts, A, B, C, and D. Part A describes basic subjects, such as units of measure, their conversion, and definition of thermophysical properties. Part B shows data of the basic solids and fluids including high-temperature melts. The periodic table and physical properties of elements are shown in Chapter B.1. A brief introduction of heat conduction, an explanation of heat capacity and thermal expansion, and a table of thermophysical properties on pure metals are compiled in Chapter B.2. Thermophysical properties of basic fluid at standard temperature and pressure are compiled in Chapter B.3. Thermophysical properties of basic fluid in a wider range of temperature and pressure are compiled in the Chapter B.4. Thermophysical properties of high-temperature melts are compiled in Chapter B.5. Part C represents thermophysical property data corresponding to various fields of application. Part D explains common information for thermophysical properties, such as uncertainty, characterization of materials, retrieval methods of thermophysical property data, thermophysical property database, molecular simulation, prediction methods, measurement methods, measurement standards, metrological standards, and a list of reference materials.

***2.3. Access to Data.*** To find specific thermophysical property data of interested materials from this handbook, they can be searched by their names and synonyms from the material name index of the handbook. Thermophysical properties of some set of materials belonging to a specific group can be accessed from a corresponding chapter or a section (for example, B.2.1, thermophysical property of pure metal; B.5.2, thermophysical property of molten salt; C.10.11, thermodynamic and transport properties of refrigerant mixtures).

Thermophysical property data required for one specific field of application can be found directly from the chapter name in part C where 15 major fields of scientific or industrial applications are specifically listed.

For most cases, the data sources, namely, references, recommended equations, or databases of thermophysical property data, can be traced back.

A detailed description of thermophysical property databases is given in the list including URL information of the website of the database.

Introductory approaches of prediction methods of thermophysical properties are explained in part D.

In this handbook, explanations of uncertainty are given in D.1 and of characterization in D.2. In the case of solid materials, it is often important to find such specifications as composition, moisture content, structure (macro, micro, nano, etc.), and thermal treatment of the material, even the product or commercial name is specified to identify the material. Basic techniques of thermophysical property measurements are explained. The International Organization for Standardization (ISO) and Japan Industrial Standard (JIS) of thermophysical property measurements are listed.

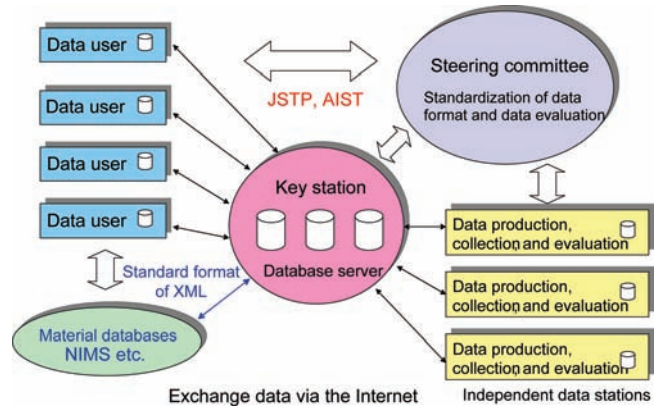


**Figure 1.** Network database system for thermophysical property data.

Reliability of thermophysical property measurements can be confirmed by measuring reference materials.[21–23] Information on available thermophysical property reference material is given.

A list of examples of laboratories or institutions for thermophysical property measurement service in Japan is given at the end of the handbook.

## 3. Database Network

***3.1. Development of Network Database.*** Databases stored with a large number of pre-examined data sets are absolutely useful to many users engaged in science and technology. Extensive collaboration among established organizations is necessary to develop such a database.[21–23] However, existing conventional databases were those of so-called concentrated type. It is common that one organization plays the role of a data center and is responsible for all management including maintenance of the database server, registration and updating of data, and improvement of database management system.

In the present case, AIST has proposed the concept of a network database system for thermophysical property data.[24] As shown in Figure 1, in the network database system, organizations contribute to the development of the database, keeping independent databases at different organizations, each of which works for registering and updating thermophysical property data for the responsible field or the responsible substance or material.[24]

***3.2. Networking Database System for Thermophysical Property.*** Materials are classified into hierarchical structure in the developed network of the thermophysical property database system, and thermophysical property data are stored into the corresponding material folder in this structure.[24] Thus, information about materials and information about thermophysical properties can be stored separately in this database. The scope of the materials stored in the database can be recognized by this hierarchical structure. This structure enables users to search for the target material, following the hierarchical structure from the higher class to the lower class, in addition to the regular search procedure by keywords. Information can be obtained more efficiently following the hierarchical structure.

As shown in Figure 2, hierarchical classifications of substances or materials are displayed with a Microsoft Explorer-like appearance and can be operated by graphical user interface.

The highest level is named "domain" and classified into "Fluids" and "Solids and Melts" since many materials are used in both phases of gas and liquid, such as working fluid for energy

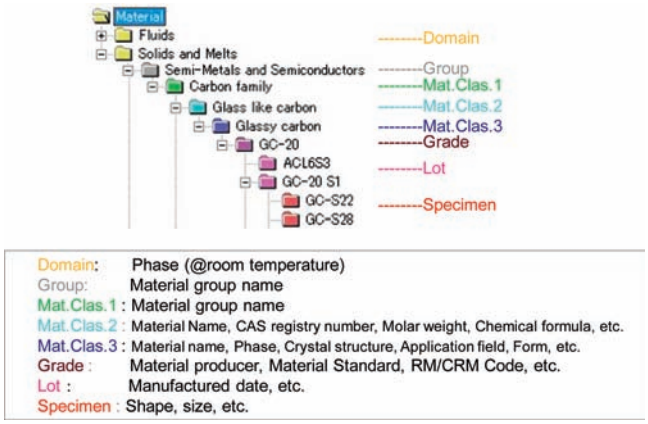


**Figure 2.** Hierarchical classifications of materials of the *Thermophysical Property Database*.

technology which vaporizes from liquid phase to gas phase and condenses from gas phase to liquid phase. On the other hand, most metals and semiconductors are solidified from melt phase. This classification is made from the viewpoint of industrial application of materials rather than the three domains of gases, liquids, and solids based on physics.

The class of the second layer is named "group", and classification lower than the groups is optimized dependent on the group.

Typical hierarchical structure for solids is as follows:

Group usually corresponds to academic or technical societies for the corresponding material group. Examples of groups are metals, ceramics, semiconductors, and polymers under the "Solids and Melts" folder.

The third level is named as "Material Class 1". Examples of Material Class 1 are oxides, carbides, and nitrides under the ceramics folder.

The fourth level is named as "Material Class 2" where substance name is stated with the information of chemical composition, IUPAC name of main component, and CAS Registry Number. Examples of Material Class 2 are aluminum oxide and silicon oxide under the oxide folder.

The fifth level is named as "Material Class 3" where the material name is stated with the information of crystalline or noncrystalline structure and micro structure. If the main component is single crystal or polycrystal, the crystal system is specified by the space group. Examples of Material Class 3 are quartz and fused quartz under the silicon oxide folder. A prediction equation for thermophysical properties of mixtures can be registered to this level, and dependence on compositions of constituent substances can be displayed.

The sixth level is named as "Grade" where the grade name of the material is stated with the information of product name, material producer, composition, and so forth. Examples of grade are POCO AXM 5Q1, IG 110 under the high density isotropic graphite folder. An equation of thermophysical property based on parameters such as Residual Resistivity Ratio (RRR) for metals can be registered to this level.

The seventh level is named as "Lot" where the lot name is stated with the information of lot characters and heat treatment.

The eighth level is named as "Specimen" where the specimen name is stated with the information of dimensions such as thickness and diameter for disk-shaped specimen, machining method and procedure for specimen preparation, surface finish, specimen characters, and heat treatment.

Since the thermophysical property of each specimen is measured, data obtained by individual measurements are registered to specimen folders at the eighth level. After a series of measurements was completed for a set of specimens of the same lot, the obtained set of data for the lot had been analyzed and evaluated, and the representative data for the lot was presented, it can be registered to the lot folder at the seventh level.

Catalogue values of thermophysical properties given to specific grades of commercial materials by manufacturers are registered to the grade folder at the sixth level. Certified values for reference materials are also registered to the grade folder.

If a thermophysical property is presented to a general substance name such as "fused quartz" without detailed information of the material enough to identify grade level, thermophysical property values can be registered to the general material name at the fifth level. Although identification of the material is not enough to specify the thermophysical property precisely and accurately at this level, the majority of currently available thermophysical property data especially for solids might be assigned to this level. This situation is also applied to most thermophysical property data of solids recorded in published data books including the *Thermophysical Property Handbook*.

In this database, thermophysical property data are registered to the folders located between the fifth level and the eighth level. Identification of the material for individual thermophysical property data by measurement is clear if the data are registered at lower levels "Specimen" and "Lot".

***3.3. Data Category.*** In this database property data are classified into the "Data" category viewed from three dimensions: "Data type", "Traceability", and "Authorization", as shown in Table 1.

The first dimension of the data category is "Data Type". Users often want to know the origin of the data and also the process such as how the data was produced or whether the data was measured, derived from the relationship between other known physical properties, synthesized by curve fitting, calculated by numerical simulation, or predicted in value by material physics.

The second dimension of the data category is "Traceability". Traceability refers to the measured data and the original measurement data from which data are derived or synthesized. The term Traceability is used to show an unbroken chain of explanation relating the method and the instrument of measurement to one established standard. Calibration to a traceable standard can be used to determine an instrument's bias, precision, and accuracy. In many countries, national standards for units are maintained by a National Measurement Institute (NMI). To obtain universal physical property values independent of individual instruments, the measurement should be traceable to the national standard or, if the national standard has not been established, some other reliable standard. Thus, the levels for Traceability are international standard, national standard, industrial standard, and other standard traceable to established standard. If the measurement is traceable to the national standard, uncertainty can be certainly given for the measured data. This database can record uncertainty to each data if available. Information of uncertainty definitely guarantees reliability and value of the data.

The third dimension of data category is "Authorization", how and by whom the data was authorized. The data reported on a reviewed scientific journal can be thought as authorized by the reviewers and the editorial board of the journal. CINDAS has recommended much thermophysical property data. National metrology institutes can supply certified reference materials, and certified values of thermophysical property are given to them.

**Table 1. Three Dimensions of Data Category and Their Attributes**

| Data Type | | Traceability | | Authorization | |
|---|---|---|---|---|---|
| attribute | definition | attribute | definition | attribute | definition |
| 1. measured | measured value | 1. industrial standard | measure based on industrial standard | 1. reviewed journal | data from reviewed journal |
| 2. derived | derived from other physical properties using physical law | 2. national standard | value of national standard | 2. provisional | preliminary data or data in progress |
| 3. synthesized | derived from curve fitting or synthesizing data of the same property | 3. standard | value of standard | 3. recommended | recommended by an organization |
| 4. simulated | predicted value by numerical simulation | 4. traceable | values obtained by traceable measurement | 4. certified | certified by an authorized organization |
| 5. theoretical | predicted value by physics | 5. unknown | values obtained by measurement of unknown traceability | 5. catalogue | material producer's data |
| 6. others | all other data | 6. others | all other data | 6. evaluated | evaluated by the steering committee of the database |
| | | | | 7. others | all other data |

Producers of materials supply their products with thermophysical property values written in catalogs. The steering committee of the database has a plan to evaluate the data and to give evaluated values.

***3.4. User Interface.*** Browsing software called as TPDS-web and InetDBGV has been developed to access the database via the Internet. TPDS-web enables us to access database very easily without user registration (it needs only a contents license agreement) and software installation.

TPDS-web can be accessed at the following URL: http://riodb.ibase.aist.go.jp/TPDB/DBGVsupport/English/.

JSTP members can browse the *Thermophysical Property Database* also at the following URL: http://jstp.mech.nagasaki-u.ac.jp/TPDS-web/index.aspx.

InetDBGV has a much more intelligent and versatile user interface than TPDS-web. The latest version of it can be downloaded from the following URL: http://www.aist.go.jp/RIODB/TPDB/DBGVsupport/.

As shown in Figure 2, the network database of thermophysical property classifies the stored thermophysical property data into a hierarchical structure of materials. Such a structure can record physical properties as "files" under the "folder" of material, much like Explorer. The hierarchy classification of materials can be updated flexibly by the structure. When the graph is clicked, detailed information such as numeric data, material information, and reference is provided. Plots of different materials can be displayed on the same figure by a drag-and-drop operation.

***3.5. Search.*** According to this classification of materials, the target materials can be found from higher level to a lower level without using the search engine. When the search engine is applied to such a hierarchical structure, information can be accessed more quickly by simple keywords as shown in Figure 3.

Two search functions "Material Search" and "Property Search" are ready. It is possible to search satisfying both conditions at the same time. Material name, chemical formula, material code (CAS registry number), and so forth can be retrieved by Material Search. Materials having physical property values of specified range can be retrieved for materials utilization and system design. Figure 3 shows search results for the word "SUS" from the network thermophysical property database simultaneously connected to AIST server and JSTP server.

***3.6. Data Stored into the Database.*** This database accumulates thermophysical property data such as thermal conductivity, specific heat capacity, thermal expansion coefficient, surface tension, viscosity and density, and so forth for a variety of materials including solids, high temperature melts, and fluids. At present, thermophysical property data of (1) standard and basic data, (2) functional materials, (3) reference data of fluids and high temperature melts, (4) thin films and boundary thermal resistances, (5) materials for use at high temperatures, (6) materials for use at low temperatures, and (7) organic materials and inorganic materials are stored in the database server of AIST. A list of contents is shown in Table 2.

## 4. Examples of Collaboration between the Handbook and the Database

***4.1. Access to the Handbook Data via the Database.*** The JSTP and Yokendo Co. Ltd., the publisher of the *Thermophysical Property Handbook*, signed the memorandum of understanding that the data on the handbook can be stored into the database server of JSTP, and the members of JSTP are allowed to view the graph of the data on the handbook. Data stored in JSTP server and in AIST server can be accessed at the same time and displayed on the same graph by using the browsing software InetDBGV as shown in Figure 4.

***4.2. Internet Access of Data and Feedback from the Users.*** Normally, the data book or the handbook will be revised after period of five years or longer. The policy guideline for revision, such as priority of the data categories to be added, is determined in the academic society or the editorial committee of the book based on supply-side information. Direct needs from user-side for physical property data can be obtained from the access record of the database. Data users can request needed data which they could not find in the database from the key station of the database interactively. Thus, the contents of the database can be updated reflecting the user-side needs. Eventually, the policy guideline for revision of the handbook can be decided on the basis of the accumulation of this information from the data users.

***4.3. Graphical Display of Equations.*** To obtain a thermophysical property value at a specified condition such as temperature or to supply data to simulation software, a function which interpolates the data points is required. This is the most classical way in this kind of collaboration, and a number of basic points to lead possible mistakes can be checked. There might be the existence of phase change temperature, structure transition, chemical reaction, inner transfer of moisture, and so on. Some properties, such as liquid viscosity, show very steep change against temperature or composition, and delicate correlation analysis is needed.

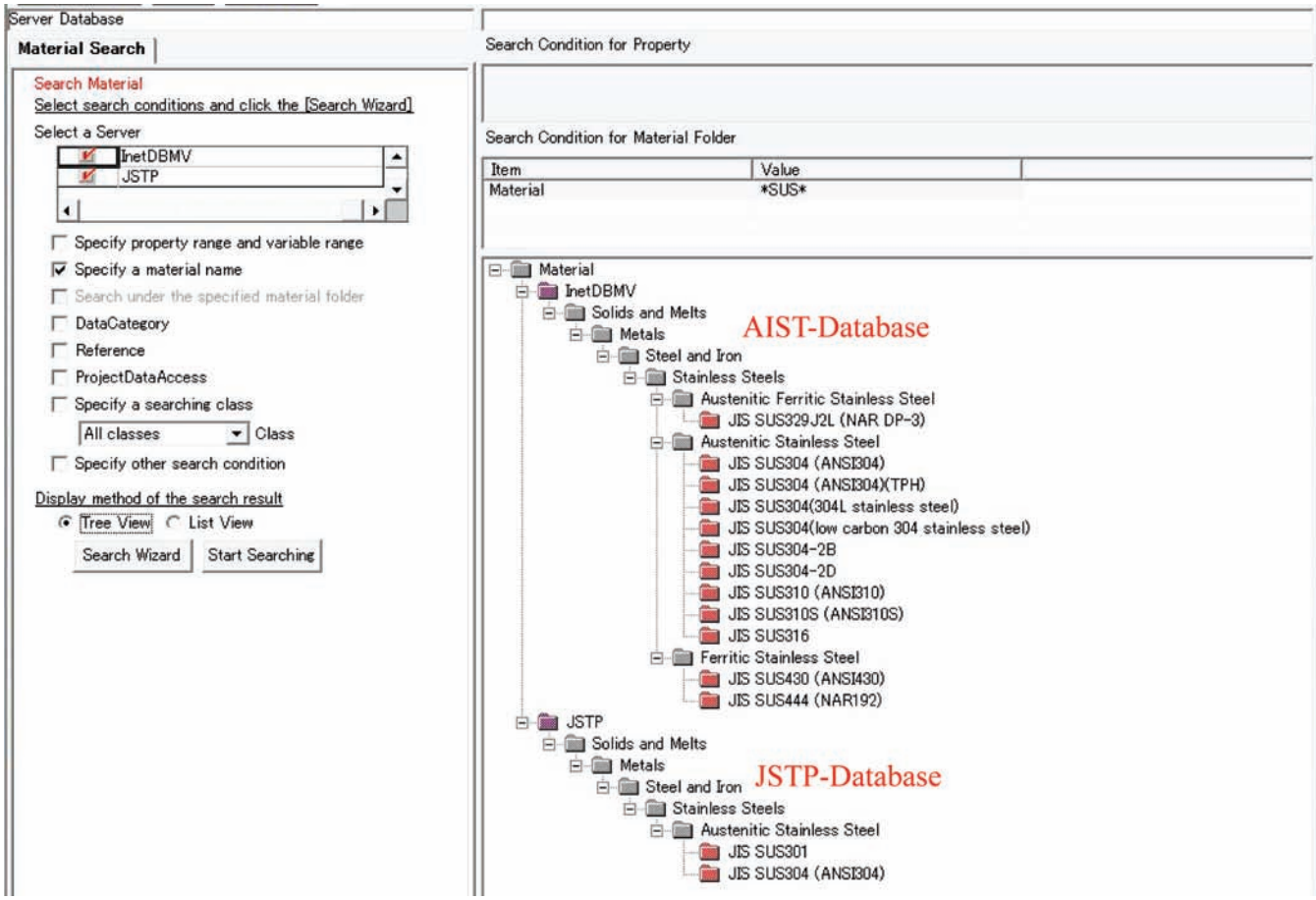


**Figure 3.** Search results for the word "SUS" from the network thermophysical property database simultaneously connected to AIST server and JSTP server.

**Table 2. List of Stored Data in the *Thermophysical Property Database* of AIST**

| material | number of data | material | number of data |
|---|---|---|---|
| alkanes and alkane halides | 1262 | metals | 1046 |
| N-containing compounds | 884 | ceramics | 145 |
| aromatic compounds | 622 | semi-metals and semiconductors | 124 |
| esters (a) mono-carboxylates | 536 | slags and molten salts | 83 |
| alcohols | 534 | thin films | 67 |
| inorganic materials | 342 | nonmetallic elements | 55 |
| aldehydes and ketones | 329 | polymers | 48 |
| S-containing compounds | 292 | other compounds | 19 |
| alkenes and alkynes | 281 | glasses | 6 |
| esters (b) di-caroxylates | 258 | total | 1593 |
| cyclo-alkanes and -alkenes and spiro-alkanes | 237 | | |
| ethers | 220 | | |
| esters (c) unsaturated carboxylates | 183 | | |
| organometallic compounds | 179 | amount of property data = 9125 | |
| natural refrigerant | 33 | | |
| water | 3 | | |
| total | 7532 | | |

The functions given in the handbook are stored in the *Thermophysical Property Database* of JSTP and can be retrieved and displayed graphically. For example, thermal expansion of ceramics is given as third-order polynomial functions, and sets of the coefficients of the functions are tabulated on pages 283 to 287 in the handbook.[17] Although numerical values for a limited number of temperatures are given in the handbook, detailed numerical tables with finer temperature pitch and graphic displays for thermal expansions can be prepared easily by collaborating with the computer database as shown in Figure 5.

When any new data of thermal expansion are added, revised regression data can be produced efficiently and promptly by fitting them to the functions using the database utility. These updated data can be published in the future edition of the *Thermophysical Property Handbook*.

Other examples of collaboration between the handbook and the database are introduced in the Appendix.

## 5. Necessity of Data for New and Advanced Applications

So that both processes work for the new handbook and the networking databases system, an extensive search of available data was performed, and lack of available data was realized in certain fields.[25]

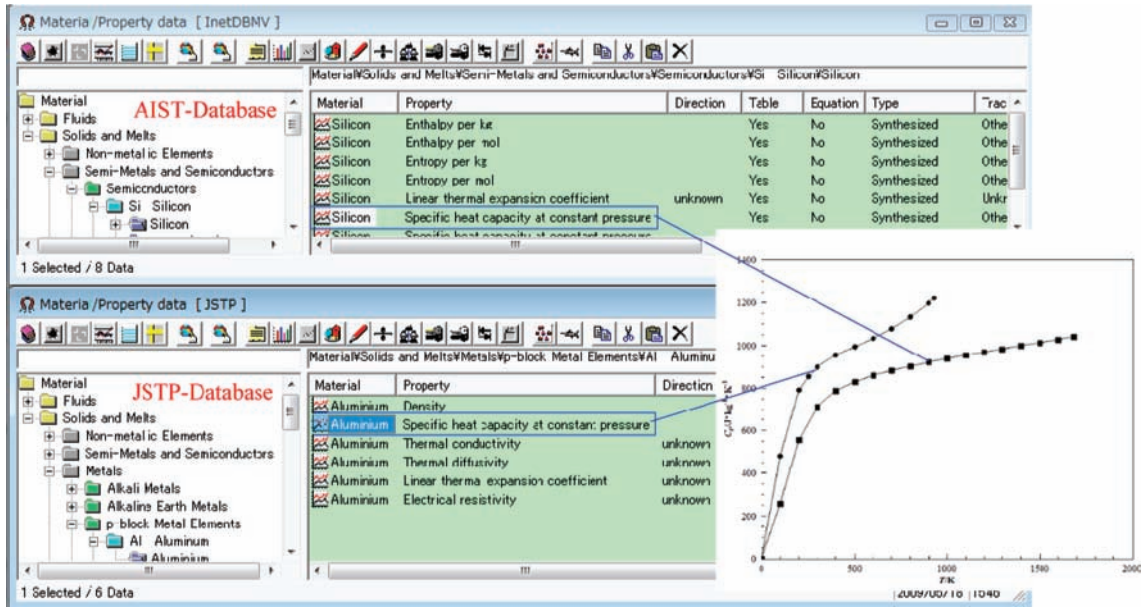


**Figure 4.** Display of the graphical user interface of the network thermophysical property database simultaneously connected to AIST server and JSTP server. The figure shows temperature, $T$, dependence of specific heat capacity at constant pressure, $C_p$, for ●, Al; ■, Si.

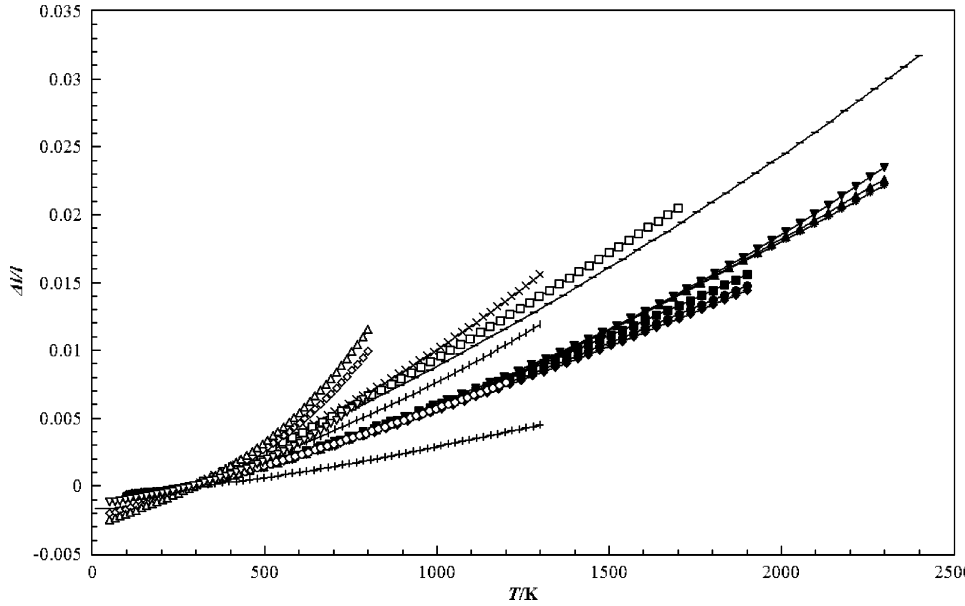


**Figure 5.** Temperature, $T$, dependence of linear thermal expansion, $\Delta l/l$, for ceramics. ●, $Al_2O_3$ single crystal; ■, $c$-axis of $Al_2O_3$ polycrystal; ◆, $a$-axis of $Al_2O_3$; ▲, BeO polycrystal; ▼, $c$-axis of BeO single crystal; ∗, $a$-axis of BeO single crystal; −, CaO polycrystal; |, GeO polycrystal; +, $c$-axis of GeO single crystal; ×, $a$-axis of GeO single crystal; ○, $In_2O_3$ polycrystal; □, MgO polycrystal; ◇, $SiO_2$ polycrystal; △, $a$-axis of $SiO_2$ single crystal; ▽, $c$-axis of $SiO_2$ single crystal.

Necessity of more data infra has been realized especially for new fields for advanced technology. A systematic approach is urgently needed, for example, in the following fields: (1) data of environmentally concerned materials such as wastes and deteriorated materials, (2) new material composites, new glasses, nanomaterials, and so forth, (3) agricultural materials, biomedical materials, foods, human tissues, and so forth, and (4) data on change due to moisture content, composite structure, and so forth.

To cover these needs, a simulation procedure in collaboration of the handbook and the database is also one possibility. Some of the above-mentioned items are specifically explained here.

***5.1. Thin Films.*** Thermophysical properties of thin films have attracted the interest of scientists and engineers in the modern research fields related to microelectronics and nanotechnologies. Transport properties such as electrical resistivity, thermal conductivity, and thermal diffusivity of thin films are known to be dependent on the synthesis process in many cases. It is necessary to investigate the relationship between the transport properties and the nanoscopic structure of thin films systematically to understand thermophysical properties of thin films, which might be different from those in bulk materials having the same chemical composition.[26]

***5.2. Carbon Materials.*** Carbons have a variety of structures, such as graphite, diamond, carbine, glassy carbon, carbon fiber, carbon nanotube, fullerene, and so forth. Therefore, carbon materials are typical examples which are difficult to give universal thermophysical property data independent of specimens. In the case of graphite, transport properties such as electrical resistivity, thermal conductivity, and thermal

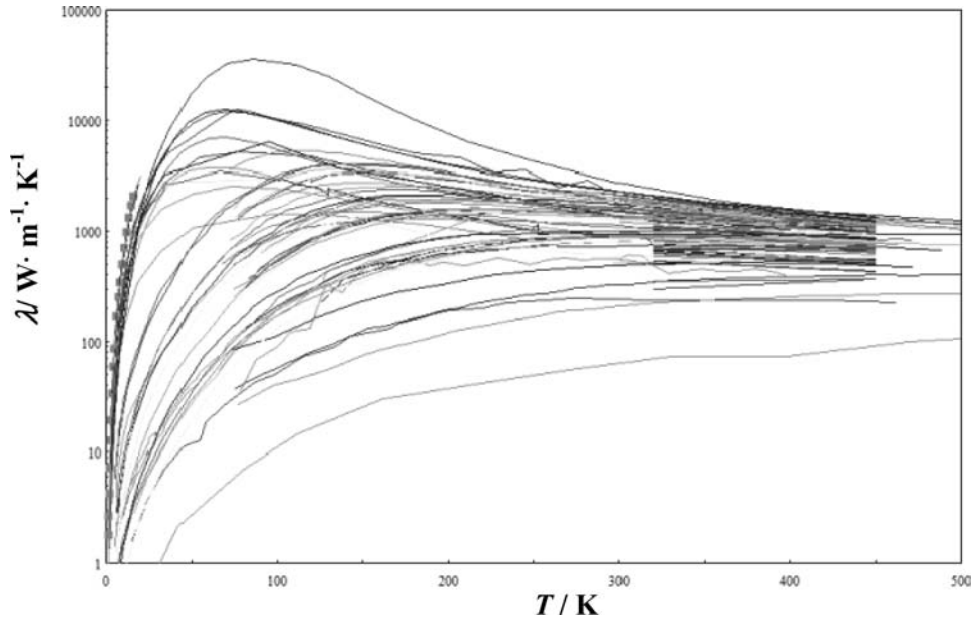


**Figure 6.** Graphical display of temperature dependence of thermal conductivity, $\lambda$, of bulk diamond and CVD diamond stored in the *Thermophysical Property Database*.

diffusivity are dependent on their microscopic structure over a wide temperature range. These transport properties are more sensitive to the structure than to the chemical composition. The structure of graphite is changed by heat treatment. In the case of carbon nanotube, the reported thermal conductivity value of carbon nanotube is different by more than 100 times depending on literature.[27] There are two major reasons for these differences. One reason is the difference of the materials even if they can be called by one name such as a carbon nanotube (single wall, multiwall, metallic, semiconductor, singe isolated tube, bundle of tubes, forest, etc.). In this case, reasonable characterization of the materials is urgently needed. Another reason is uncertainty of measurement methods. To solve this problem, traceability and critical evaluation of the measurement methods are needed.[22,28]

Diamond is known as the highest thermal conductive material and important as a heat spreader for electronics and optoelectronics where temperature rise induced by extremely dense heat generation is a serious problem. Although three types of diamond, I, IIa, and IIb, are known, the thermal conductivity of bulk diamond is not so diverse as graphite or a carbon nanotube. Thermophysical property data of diamond films and nano diamond films synthesized by chemical vapor deposition, and so forth, are added to the database and compared with those of bulk diamond. Figure 6 shows a graphical display of temperature dependences of thermal conductivity values of bulk diamond of different grades and chemical vapor deposition (CVD) diamond synthesized under variety of conditions stored in the *Thermophysical Property Database*. Research has been started to create a data set for the thermal conductivity of diamond from these data utilizing multiple functions and a graphical user interface prepared by the database. The information can be fed back to synthesized diamond films for the required property.

When this analysis by the database is successful for not only diamond but also graphite and carbon nanotube and so forth, a systematic presentation of the thermophysical property data of them is possible as shown in the handbook and the database.

***5.3. Collaboration on Thermophysical Property Data.*** As described in the introduction, activities by the IUPAC subcommittees, the IACT, and the IATP in the past and present are excellent examples of the international collaboration of experts for critical evaluation of experimental data under the leadership of Professor W. A. Wakeham for many years.[7–9,29] For some of the specific substances, efforts by experts, for example, International Association for Properties of Water and Steam, have made a substantial contribution to the critical evaluation of thermophysical property data.[29,30]

It has been pointed out that a common format will enhance efficient exchange and sharing of these evaluations on thermophysical property data. As described in the introduction, *ThermoML: XML-Based Standard for Data Storage and Exchange* as a standard format for data storage and exchange was developed by TRC, mainly concerning fluid properties which are well-characterized by composition and impurities.[15]

On the contrary, to characterize solid materials, diverse and hierarchical information, such crystal or noncrystal structures, microstructures, or composite structures, and so forth, must be specified. Therefore, a rational structure of the database and common format for properties of solid materials should be different from those for properties of fluids.

One trial approach to develop a common format for properties of solids has started as a collaborative research to establish a common approach based on XML under the scheme of the Intellectual Infrastructure Project in Japan. Related to this format, a task group for "Exchangeable Materials Data Representation to Support Scientific Research" was approved by the CODATA 25th General Assembly, Beijing 2006.[31]

Modern information technology represented by the computer and communication technology realized drastic progress for huge supply and efficient use of thermophysical property data. One unexpected problem realized in the process is that the data "once-killed" by critical evaluation often comes back by modern searching technology and used carelessly in

applications. It is an urgent issue to start organizational efforts to solve this "revival of once-killed data" problem.

## 6. Concluding Remarks

Function sharing and a collaborative approach between printed media and computerized database are important subjects for future study. Through the work for both the *Thermophysical Properties Handbook* and the networking database, the present authors realized this importance and expressed introductory findings in the present paper. The conceptual idea and some trials are explained, although they are in their early stage. It was also pointed out that the organizational efforts are needed for critical examination of materials data, for confinement of "once-killed" data, and for further needs of new data for particularly advanced applications.

## Appendix

Other examples of collaboration between the handbook and the database are as follows.

**Table A1. Electrical Resistivity, Thermal Conductivity, and the Lorentz Number of Pure Metals**

| | electrical resistivity | thermal conductivity | Lorentz number·$10^{-8}$ |
|---|---|---|---|
| material | $\mu\Omega$·cm | W·m$^{-1}$·K$^{-1}$ | W·$\Omega$·K$^{-2}$ |
| Li | 8.55 | 76.8 | 2.19 |
| Be | 2.8 | 280 | 2.61 |
| Na | 4.2 | 132 | 1.85 |
| Mg | 4.02 | 156 | 2.09 |
| Al | 2.75 | 237 | 2.17 |
| Ti | 57 | 22 | 4.18 |
| Ni | 7.6 | 90.5 | 2.29 |
| Cu | 1.55 | 398 | 2.06 |
| Zr | 43.3 | 23 | 3.32 |
| Mo | 5.4 | 138 | 2.48 |
| Ag | 1.61 | 427 | 2.29 |

### *A.1. Analysis of Correlation among Thermophysical Properties*

According to the Wiedemann−Franz law, the Lorentz number $L$ is defined by the following equation:

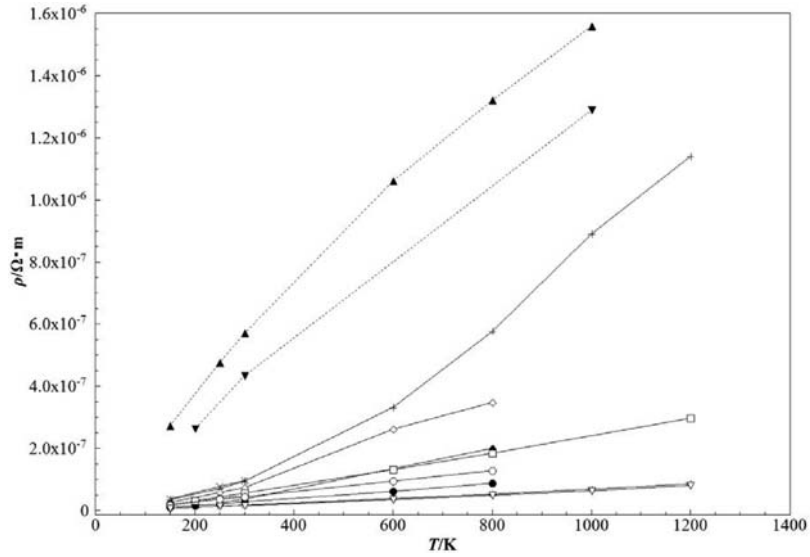


**Figure A1.** Temperature, $T$, dependence of electrical resistivity, $\rho$, of basic metals. ●, Al; ◆, Be; ∗, Cu; +, Fe, ×, Li; ○, Mg; □, Mo; ◇, Ni; ▽, Ag; ·●·, Na; ·▲·, Ti; ·▼·, Zr.

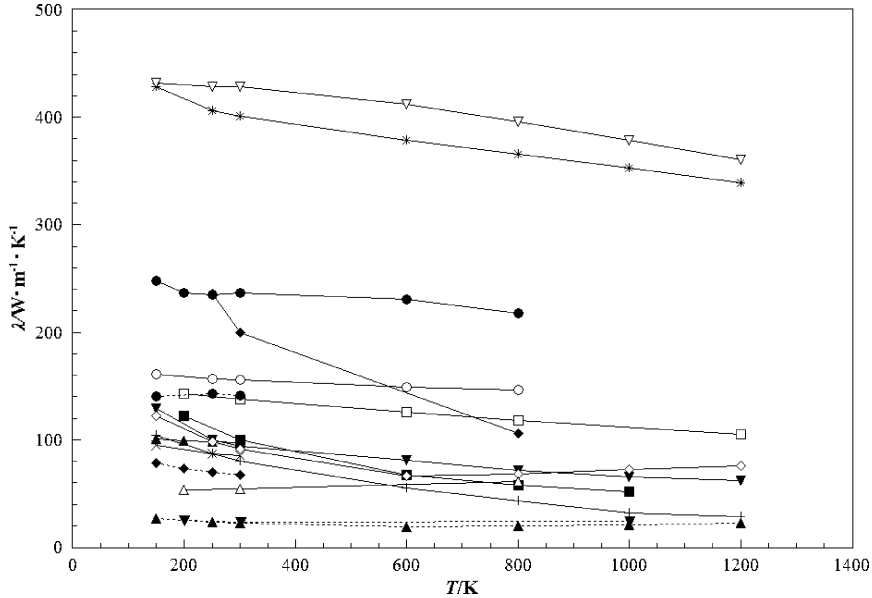


**Figure A2.** Temperature, $T$, dependence of thermal conductivity, $\lambda$, of basic metals. ●, Al; ◆, Be; ▲, Cd; ▼, Cr; ■, Co; ∗, Cu; +, Fe; ×, Li; ○, Mg; □, Mo; ◇, Ni; △, Nb; ▽, Ag; ·●·, Na; ·◆·, Sn; ·▲·, Ti; ·▼·, Zr.

$$L = \lambda\rho/T \qquad \text{(A1)}$$

where $\lambda$ is the thermal conductivity, $\rho$ is the electrical resistivity, and $T$ is the absolute temperature.

Table A1 shows the electrical resistivity, the thermal conductivity, and the Lorentz number of pure metals at 300 K on page 28 of the *Thermophysical Properties Handbook*.[18] Figures A1, A2, and A3 show temperature dependences of the electrical resistivity, the thermal conductivity, and Lorentz number of these metals calculated by eq A1. The horizontal broken line in Figure A3 indicates the ideal value of the Lorentz number based on the free electron model by the Drude theory ($2.44 \cdot 10^{-8}$ W·Ω·K$^{-2}$). Figure A3 demonstrates that the difference of Lorentz number for basic metals is smaller than 30 % at higher temperatures over 600 K, whereas the electrical resistivity and the thermal conductivity deviate more than 10 times depending on materials, as shown in Figures A1 and A2, respectively. At higher temperatures than 600 K, plots of magnesium, aluminum, copper, and silver are close to the ideal value of the Lorentz number. The plots of other metals are higher than the ideal value. Since this figure gives more extensive information than Table A1 which tabulates only the values at room temperature, it can be used as a tool for data evaluation based on the consistency of relation among thermophysical properties.

### *A.2. Data Set*

Figure A4 shows thermal conductivity values of pure irons, carbon steels, and stainless steels at temperatures displayed on page 29 of the *Thermophysical Properties Handbook*.[18] The temperature dependence of the thermal conductivity is explained by heat conduction carried by free electrons for pure irons. In the case of carbon steels as interstitial alloys, the temperature dependence of thermal conductivity can be explained by free electron transport scattered by local lattice deformation induced by interstitial atoms. In the case of stainless steels as substitutional alloy, the temperature dependence of thermal conductivity can be explained by of free electron transport

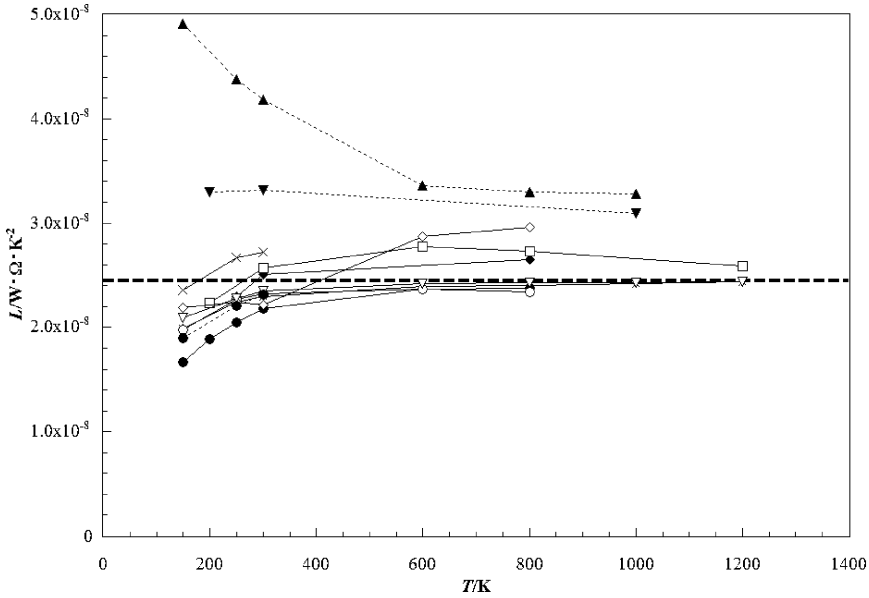


**Figure A3.** Temperature, $T$, dependence of Lorentz number, $L$, of basic metals. Thick dashed line, ideal value; ●, Al; ◆, Be; ∗, Cu; ×, Li; ○, Mg; □, Mo; ◇, Ni; ▽, Ag; ·●·, Na; ·▲·, Ti; ·▼·, Zr.

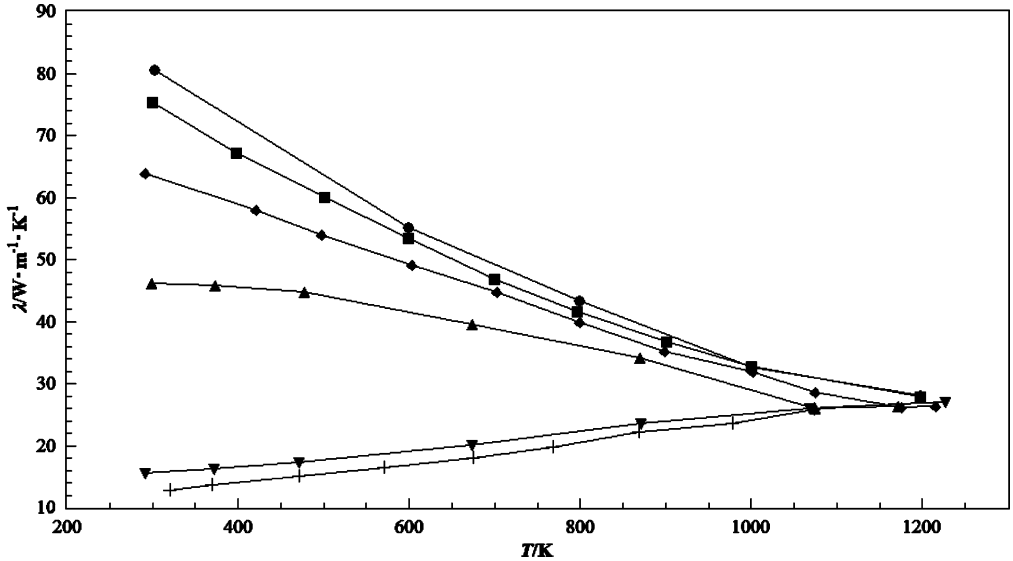


**Figure A4.** Temperature, $T$, dependences of thermal conductivity, $\lambda$, of pure irons, carbon steels, and stainless steels in the *Thermophysical Properties Handbook*: ●, pure Fe, example 1; ■, pure Fe, example 2; ◆, carbon steel (C, 0.1 %; Mn, 0.5 %); ▲, carbon steel (C, 0.23 %; Mn, 1.5 %);▼, stainless steel (Cr, 18 %; Ni, 8 %); +, stainless steel (Cr, 18.4 %; Ni, 9.6 %).

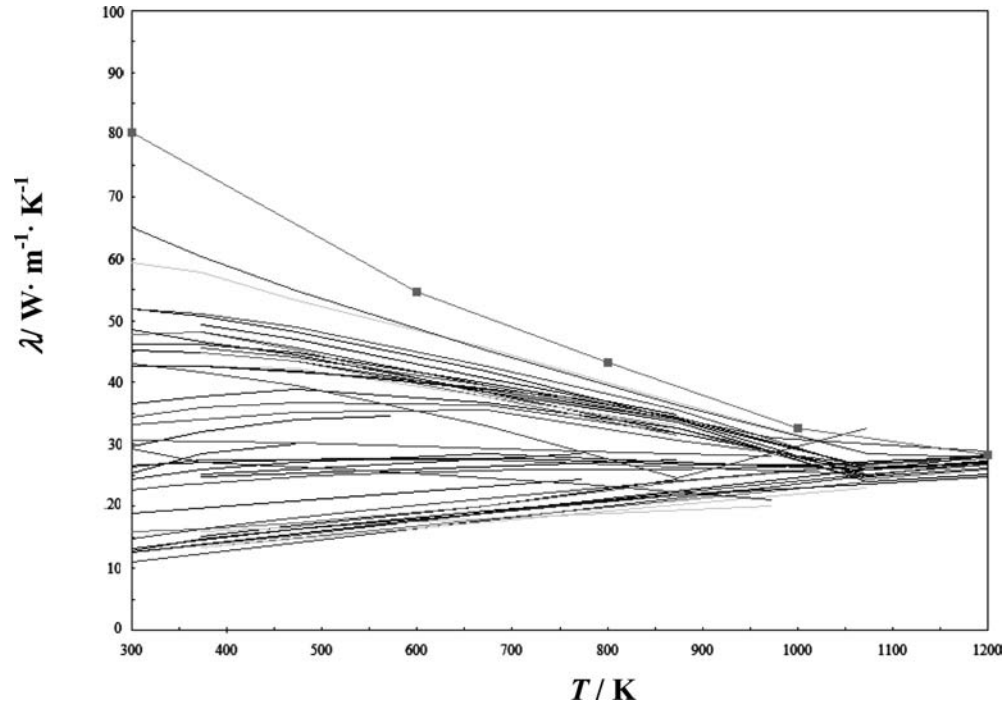


**Figure A5.** Graphical display of the temperature dependences of the thermal conductivity, $\lambda$, of pure irons, carbon steels, and stainless steels stored in the *Thermophysical Property Database*.

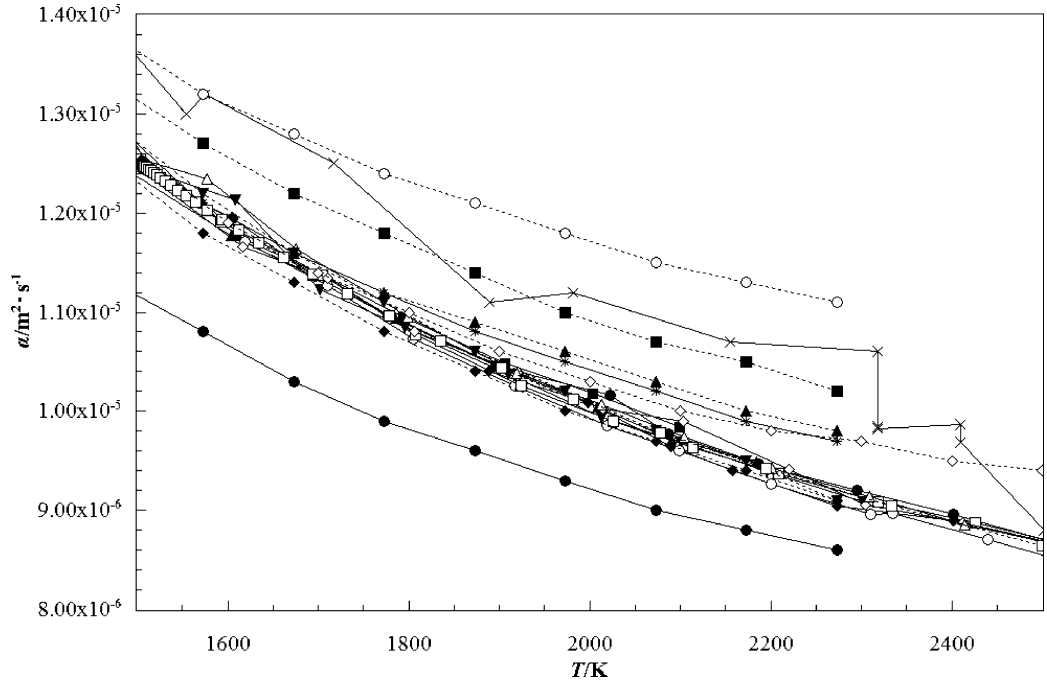


**Figure A6.** Temperature, *T*, dependence of the thermal diffusivity, α, values for RM 8424-8426 (black square plots) together with those of POCO AXM-5Q1 graphite and 5Q graphite reported in literature. ●, 035-1; ■, 035-1-2; ◆, 035-2; ▲, 035-2-2; ▼, 035-3; ○, 035-3-2; □, 035-4; ◇, 035-5; △, 035-6; ▽, 102-1; ×, 102-2; |, 401-1; ·●·, no. 255; ·■·, no. 260; ·◆·, no. 261; ·▲·, no. 262; ·▼·, no. 266; ·○·, no. 269; ·□·, RM 8424-035; ·◇·, RM 8424-8426.

scattered by screened Coulomb potential induced by substituting ions. Since data points plotted in this figure are rather limited, there is not enough information to know the spread of thermal conductivity for different grades of carbon steel or stainless steel, respectively.

Figure A5 shows a graphic display of temperature dependence of thermal conductivity data over pure irons, carbon steels, and stainless steels stored in the *Thermophysical Property Database*. Important information observed in Figure A5 is the continuous change of thermal conductivity from pure iron via carbon steel to stainless steel. On the basis of this information, it might be possible to derive a general formula to express the temperature dependence of the thermal conductivity universal for pure irons, carbon steels, and stainless steels, and Figure A4 in the second edition of the *Thermophysical Properties Handbook* can be updated in the next edition of the handbook. As shown in this example, the database accelerates renovation of the handbook, and the handbook publicizes the updated information to general users of science and technology.

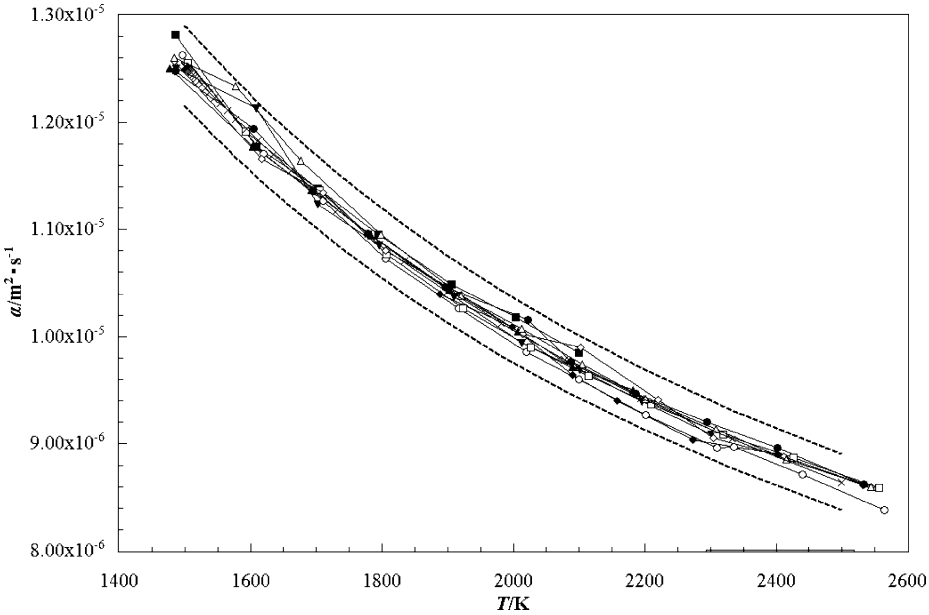


**Figure A7.** Fitted function of the thermal diffusivity, α, values for RM 8424-035 (black plots) with uncertainty of 3 % region (between broken curves) together with those of measured plots. ●, 035-1; ■, 035-1-2; ◆, 035-2; ▲, 035-2-2; ▼, 035-3; ○, 035-3-2; □, 035-4; ◇, 035-5; △, 035-6; ×, RM 8424-035.

### *A.3. Data Evaluation for Reference Material*

The laser flash method is considered as the most reliable method for measuring the thermal diffusivity of solid materials at temperatures above 1500 K.[32] However, for practical use of this method in industry, there is a need for reliable reference materials for the thermal diffusivity.

One of the candidate reference materials for the thermal diffusivity at high temperatures up to 2000 K is POCO AXM-5Q1 graphite. Round-robin measurements of the thermal conductivity and the thermal diffusivity of POCO AXM-5Q graphite, which is a POCO grade of slightly lower purity than AXM-5Q1, were conducted under the auspices of the Air Force Materials Laboratory/Advisory Group for Aerospace Research and Development (AFML-AGARD) in the period of 1965 to 1972. In addition to them, several leading laboratories participated in a cooperative project under the auspices of CODATA and carried out measurements of the thermal diffusivity of POCO AXM-5Q1 graphite.

NIST is supplying POCO AXM-5Q1 as thermal conductivity reference materials, RM 8424-8426. The thermal diffusivity values for them are calculated from the reference value of thermal conductivity, specific heat capacity, and density.[33] The first edition of *Thermophysical Properties Handbook* gave thermal diffusivity values for RM 8424-8426 when density is 1730 kg·m$^{-3}$ and the electrical resistivity is 14.5 $\mu\Omega$·m.[20] Figure A6 shows the temperature dependence of the thermal diffusivity values for RM 8424-8426 together with those of POCO AXM-5Q1 graphite and 5Q graphite reported to journals and stored into the database. Thermal diffusivity data scatter more than 20 % peak-to-peak among different reports.

One of the authors, Baba, performed accurate measurements of the thermal diffusivity of POCO AXM-5Q1 graphite supplied by NIST as RM 8424-035 of which density is 1738 kg·m$^{-3}$ and electrical resistivity is 15.92 $\mu\Omega$·m in the temperature range (1500 to 2500) K applying the laser-pulse apparatus developed at the NIST.[34] The measured results and the fitted function with uncertainty are shown in Figure A7. The scattering of the data is much reduced compared with Figure A6 since the specimen is cut out from the same lot of known density and electrical resistivity. All measured points are located within the range of uncertainty plus minus 3 % (coverage factor $k = 1$). After data evaluation using the graphical function and the fitting function of the database, an evaluated equation with uncertainty can be printed on the handbook, and the background data can be accessed to the database.

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