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Problems of Data Input into a Data Base for Thermophysical Properties[1]

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THERSYST is a data base especially designed for the storage, handling, and presentation of thermophysical property data. Great effort has been spent to enable the storage of the complete relevant information on the material and the experimental conditions. A modular system of evaluation programs allows one to combine measured data with any describing data, to convert stored values to others with the help of given formula, or to transform parameters to variables. Finally, all these data can be listed and plotted in many ways. An essential time factor and source of error during storage of data are produced by the extraction of the information from the literature. In many cases the kind of presentation is not appropriate for the data transfer into the data base. A form of presentation which facilitates the literature evaluation for the data input is proposed.

KEY WORDS: data base; data evaluation; thermophysical properties.

1. INTRODUCTION

The importance of material data base for all disciplines of engineering increases with the expansion of computer application to design, manufacturing, process simulation, process control, and planning of plants and wherever "computer aid" is desired. An international discussion has been initiated by the Committee on Data for Science and Technology (CODATA) to coordinate the activities in the field of computerized materials data systems and to stimulate cooperation in data-base design and management, especially for the sake of harmonization of terminology and standardization of data organization.

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The proceedings [1] of the last CODATA workshop on material data systems for engineering contain many recommendations and much information on existing material data bases.

Special data bases on thermophysical properties of solids were described by Li and Ho [2] and Araki et al. [3]. At CINDAS [2] all thermophysical properties are covered, while the system described in Ref. 3 is limited to the thermal conductivity of reference materials.

A factual data base for thermophysical properties requires special demands insofar as thermophysical properties of solid materials not only depend on their chemical composition, but also are highly sensitive, e.g., to the micro- and macrostructure of the material, to the pretreatment of the samples, etc. This is elucidated with the aid of Fig. 1, which shows the results of a retrieval with the search criterion "total emittance of zirconium dioxide."

Thirty-two data sets were found, whereby the emittance values cover the broad range between 0.3 and 0.9. In order to restrain the range to a smaller band, the data base should be able to assist in the selection of relevant data with the aid of correlations between the property data itself and the data for the description of the material and the experimental conditions.

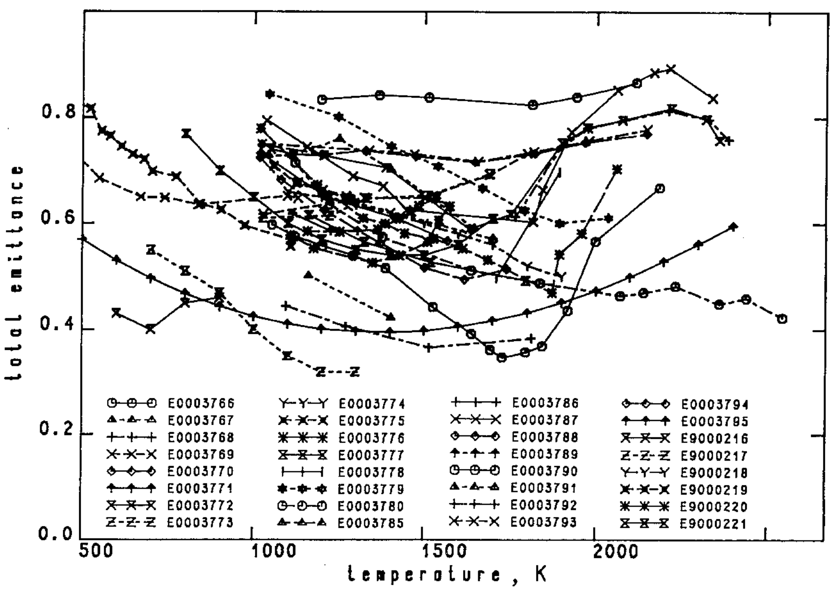

Fig. 1. Total emittance of ZrO_2. Result of a retrieval in THERSYST. The numbers (key numbers of the corresponding data sets) are listed in Table III.

Because an appropriate data-base management system for such purposes was not available, the THERSYST data base has been developed as a combination of a factual data base for thermophysical properties of solids and a modular program system to handle the data-base content. This special type of data base enables the user to find thermophysical property data for materials of his interest or, conversely, to look for materials whose thermophysical property values cover a specified range.

2. DESIGN OF THERSYST

THERSYST is based on the modular program system RSYST, which originally was developed for calculations in relation to nuclear reactors [5]. The advantage of such a system is that program components can be added or deleted in a relatively easy manner to permit an optimum configuration. Each program module can be modified without affecting other parts. The problem of the representation of the correlations between the intrinsic properties data (= thermophysical properties) and the data describing the material and the experimental technique is solved using the class concept. Each class contains a set of data objects for which identical rules of interpretation are valid.

The information, which is taken, e.g., from an original literature source, is converted to data objects of such a form. The physical content of each dataset is separated into five classes:

class 1, material designation;
class 2, material characterization;
class 3, experimental description;
class 4, thermophysical properties data; and
class 5, bibliography.

As shown in Fig. 2, classes 1 to 4 are hierarchically structured. In each level of hierarchy the next lower level is defined. The advantage of the hierarchic structure is that multiple storage of information can be reduced. For example, if more than one thermophysical property was measured for materials with identical characterizations, the content of classes 1 and 2 has to be stored only once for all these data sets; when a multiproperty apparatus is used, also the context of class 3 keeps the same. If, e.g., the thermal conductivity of a certain material was measured with varying ambient atmosphere, then the content of classes 1, 2, and 5 is the same. Thus, the user is also informed that different samples of the same material were measured by the same author. The bibliographic information is not included in the hierarchic structure but it is linked to the corresponding data set by the document number.

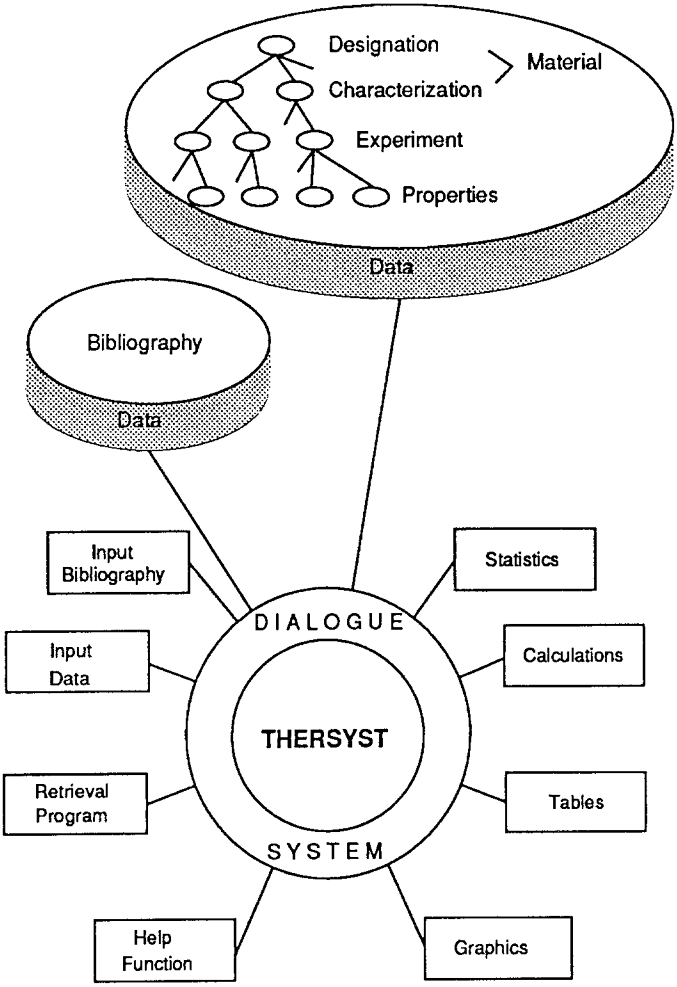

Fig. 2. Elements of the modular system THERSYST for storage, handling, and representation of thermophysical property data.

3. THERSYST DESCRIPTORS

All information belonging to a set of measurement values describing the property results itself, the material, and the measurement technique is stored in the form of descriptors. In Table I the available descriptors are listed together with the abbreviations as they are used in THERSYST. The descriptors can either be numerical (n), coded (cd), or in text form (tx). In

Table I. THERSYST Descriptors

No.	Abbreviation	Descriptor	Type
1	TABNO	Number of table or figure	n
2	COLNO	Number of column or curve	n
3	Y	Thermophysical property	cd
4	X	Variable	cd
5	YSP	Property specification	cd, n
6	DIR	Measuring direction	cd, n
7	PAR	Parameter	cd
8	ACC	Measurement accuracy	n
9	CLASS	Data classification	cd
10	YTXT	Remarks on result	tx
11	EXMET	Measurement technique	cd
12	EXAPP	Producer and type of apparatus	tx
13	EXTEM	Temperature measurement technique	cd
14	SAMPLE	Sample dimensions	tx, n
15	AGAS	Kind of ambient atmosphere	tx
16	APRES	Pressure of ambient atmosphere	n
17	EXTXT	Remarks on experiment (<400 char.)	tx
18	PNAM	Name and synonyms of the material	tx
19	MATG	Material group	cd
20	CNAM	Chemical symbol/formula	cd
21	PROD	Producer of the material	tx
22	CCOM	Chemical composition, symbols, and amount of components	tx, n
23	STATE	Physical state (solid, liquid, etc.)	cd
24	MFOM	Particular form of material	cd
25	STR	Microstructure of the material	cd
26	CSTR	Crystal structure	cd
27	SSOL	Solid solution?	
28	STRTXT	Remarks to the microstructure (<240 char.)	tx
29	PREP	Preparation technique	cd
30	TREATM	Mechanical sample treatment	cd
31	TREATT	Thermal treatment	cd, tx, n
32	TREATX	Other sample treatment	cd
33	ROUGH	Information on surface roughness	cd, n
34	LAYCOM	Composition of surface layer	tx
35	LAYTH	Thicknes of surface layer	n
36	DEN	Density at room temperature	n
37	TD	Theoretical density	n
38	POR	Porosity (vol%)	n
39	PORTYP	Type of porosity	cd
40	ERR	Electrical resistivity at $T=$?	n
41	CT	Curie temperature	n
42	DT	Debye temperature	n
43	MELTT	Melting temperature	n
44	MELTH	Heat of fusion	n
45	TRATXT	Kind of transition	cd
46	TRAT	Transition temperature	n
47	TRAH	Heat of transition	n
48	MATTXT	Remarks on material characterization (400 char.)	tx
49	AU	Author	
50	IN	Institution	
51	SO	Title, source, year of publication	

some cases the input units are optional, and mostly the units are fixed for the sake of facilitation of the input.

In Table I the descriptors are listed in an order is different from the one given by the hierarchical structure. But it is more convenient first to select individual curves out of a set of measurement curves and then to describe the corresponding information on material and experiment for each individual curve. Then the appertaining descriptors have to be given, and usually first the experiment and thereafter the material have to be described. The abbreviations in the second column in Table I are the codes as used in THERSYST.

3.1. Explanations of and Comments on the Descriptors

Nos. 1 and 2: Refer to the location of the numerical data set in the original representation

No. 3: THERSYST is dealing with the following thermophysical properties:

THC, thermal conductivity
THD, thermal diffusivity
CP, specific heat at constant pressure
CV, specific heat at constant volume
ENT, enthalpy
LEX, linear thermal expansion
VEX, volumetric thermal expansion
DEN, density
ELR, electrical resistivity
LOR, Lorenz number
ABS, absorptance
EMI, emittance
REF, reflectance
TRA, transmittance
ACO, absorption coefficient
RIN, refractive index

No. 4: Usually the temperature will be the independent variable X. But X may also be any other physical entity, figuring as THERSYST descriptor, e.g., density, pressure, wavelength (emittance), chemical composition, etc.

No. 5: For examples, *lattice* conductivity, *total spectral* emittance, *hemispherical* emittance. Here additional notes have to be made, e.g., for frequency of electrical AC resistivity measurements or reference values of thermal expansion measurements.

No. 6: Important in the case of anisotropic materials

No. 7: If the described set of measurement values is part of the parameter study, it has be noted which parameter has been varied.

No. 9: For example, original measurement points, smoothed curve, calculated from other measured properties, estimated from theory or various literature data

No. 10: Comments on the results

Nos. 11–17: Information on the experimental conditions. The measurement technique should be designated with the standard designation, if possible (e.g., guarded hot plate, laser pulse technique, drop calorimeter).

No. 18: Name(s) of the investigated material (common trade names and standard designations should also be given)

No. 19: Material group in which the investigated material has to be incorporated

Nos. 18–20: Material designation

No. 22: If the quoted component has a special function, e.g., dopant, stabilizer, or impurity, or if the material is of eutectic or stoichiometric composition, this should be noted as additional information.

No. 24.: For examples, coating, composite, foam, granule, powder, whisker, etc. Sizes of particles or diameter of fibers may also be given here.

No. 25: For example, noncrystalline, polycrystalline, multiphase, single phase, etc.

No. 26: For example, triclinic, monoclinic, cubic, etc.

No. 29: For example, Bridgman method, diffusion method, zone melting, arc cast, cold rolled, cast, hot isostatic pressed, plasma sprayed, etc.

No. 30: For example machined, polished, sand-blasted, etc.

No. 31: The atmosphere, ambient pressure, temperature, and time of thermal treatment of samples

No. 32: For example, magnetic field, irradiation, *untreated*

No. 33: Important for radiative properties. If available, the roughness factor [6] or data on root mean square (RMS), arithmetic mean roughness, etc., can be given.

Nos. 34 and 35: For example, oxide layers influencing optical properties, protective layers or coatings, the radiative properties of which are of interest

Nos. 36–39: Density descriptors

Nos. 40–47: Other material peculiarities

Nos. 49–57: With the bibliographic data, also the institution, where the measurements were carried out, should be given.

4. PROBLEMS OF PRESENTATION OF MEASUREMENT RESULTS

The aim of publication of thermophysical properties is twofold:

(a) communication of experimental results and
(b) description of the physical phenomena.

In scientific publications, emphasis is often laid on the second point. This leads to difficulties if the information needed for the data base shall be extracted by quick reading and the descriptors looked for are hidden in the text. The presentation of data is often reduced to a few diagrams, which are useful for illustration but not for reconversion to numerical values. The digitization becomes extremely inaccurate if only small figures are available, and especially if nonlinear scales are used. An additional difficulty is sometimes the identification of the individual curves of a diagram. Confusion may also be caused if the same values are plotted in several diagrams without clear comments. On the other side, if a set of curves is the result of a parameter variation, then it is often very time-consuming to find out from the text which parameter must be associated with which curve. The measurement data, and if possible the describing data, should be presented in tabular form.

For the purpose of comparison or correlation of property data from several different sources, detailed information on the material is necessary.

In every case and especially if a material analysis was not made, the author should give some notes concerning the preparation process of the sample. The measurement technique and the experimental conditions (sample geometry, ambient atmosphere, etc.) are also important for the evaluation of the results. Therefore, at least a few catchwords should be given instead, e.g., of a hint such as "reported elsewhere." For most of the commonly used measurement techniques standardized designations have been introduced [7] and these should be employed.

The transfer of all the information into a data base could be considerably facilitated if the measurement results were presented in a more or less standardized form. In the frame of such a description the numerical measurement data should be given in tabulated form. Then for every column (set of measurement values) all relevant information should be listed and guided by the descriptors in Table I. Normally most of the descriptors are identical for a couple of measurement runs, especially when parameter studies are reported. Table II shows an example of the proposed form of description. Identical descriptors are marked by dittos. The data were taken from Ref. 8 and the corresponding curves are included in Fig. 1, Table III, and (some of them) Fig. 3.

5. DATA EVALUATION BY MEANS OF THERSYST

THERSYST is a modular system combining data base and programs for

- data selection corresponding to the criteria defined by the user;
- data manipulation, e.g., conversion of units, replacement of a given variable by a new one, which was originally used as a parameter, regression of data, and calculation of a new property from stored data on other properties; and
- representation of data in the form of tables and graphs.

A detailed description of these programs is given in Ref. 4. At this place only the program VARTAB is presented, which enables us to make a problem-oriented overview of the physical content of selected curves as shown in Fig. 1. For each curve the description of material and experiment is stored according to Tables I and II. Since we know that the emittance depends mainly on the material composition, impurities, and thermal treatment (roughness is not relevant in the case of oxide ceramics), we produce a summary table showing these descriptors for all the data sets which are plotted in Fig. 1. From such a table (Table III) it can easily be seen that the composition varies between pure ZrO_2 and ZrO_2 with a high SiO_2

Table II. Proposal for a Standarized Form to Describe Thermophysical Property Results[a]

Descriptor (Table I) Code	No.	Date set				
TABNO	1	1	1	1	2	2
COLNO	2	1	2	3	1	2
Y	3	Emittance [–]	=	=	=	=
X	4	Temperature [K]	=	=	=	=
YSPEC	5	Total, hemispherical	=	=	=	=
PAR	7	Thermal treatment (TREATT)	=	=	./.	./.
ACC	8	4.8 %	=	=	=	=
CLASS	9	Original measurement point	=	=	=	=
EXMET	11	Calorimetric technique	=	=	=	=
SAMPLE	14	Layer on molybdenum, layer thickness LT = 300 μm	=	=	= LT = 60 μm	= LT = 160 μm
AGAS	15	Vacuum, 10^{-4} Torr	=	=	=	=

PNAM	18	Zirconium dioxide, stabilized, industrial material Type No. MPTU 43-57-53	=	=	= Type No. TU-ShchL0-027.241	= Type No. CHMTU 05-29-67
CNAM	20	ZrO_2, CaO	=	=	ZrO_2, SiO_2	ZrO_2, SiO_2
CCOM (wt %]	22	ZrO_2: 92.93 Balance (B)	=	=	ZrO_2: 82.3 (B)	ZrO_2: 66.0 (B)
		CaO: 5.8 Stabilizer (S)	=	=	SiO_2: 10.0 (S)	SiO_2: 33.15 (S)
		SiO_2: 0.2 Impurity (I)	=	=	CaO_2: 6.9 (S)	Al_2O_2: 1.6 (I)
		TiO_2: 1.0 Impurity (I)	=	=	Al_2O_3: 0.6 (I)	
		Al_2O_3: 0.97 Impurity (I)	=	=		
STR	25	Polycrystalline, multiphase	=	=	=	=
CSTR	26	Cubic (simple)	=	=	=	=
SSOL	27	Yes	=	=	=	=
PREP	29	Plasmasprayed in air	=	=	=	=
TREAT	31	Untreated	Annealed in vacuum at 1900 K	Annealed in vacuum at 2330 K	./.	./.
(EKEY)[b]		(E 003772)	(E003773)	(E003774)	(E003779)	(E003776)

[a] The information was taken from Ref. 8.
[b] Key number of the THERSYST data set.

Table III. Summary Listing Selected off Descriptors Referring to the Emittance Curves of ZrO_2, as Plotted in Fig. 1

EKEY	CCOM	CCOMA	D	TRTEM	TRATM	AU
E003766	ZrO_2	99.57 wt%	B	—		G. A. Zhorov
	SiO_2	0.2000	I			
	TiO_2	0.1000	I			
E0003767	ZrO_2	99.57 wt%	B	1625.	Vacuum	G. A. Zhorov
	SiO_2	0.2000	I			
	TiO_2	0.1000	I			
E0003768	ZrO_2	99.57 wt%	B	1920.	Vacuum	G. A. Zhorov
	SiO_2	0.2000	I			
	TiO_2	0.1000	I			
E0003769	ZrO_2	92.10 wt%	B	1125.	Air	G. A. Zhorov
	CaO	5.800	S			
	Al_2O_3	0.5600	I			
E0003770	ZrO_2	92.00 wt%	B	—		G. A. Zhoroov
	SiO_2	0.2000	I			
	HfO_2	1.000	I			
En003771	ZrO_2	92.00 wt%	B	1375.		G. A. Zhorov
	CaO	5.800	S			
	HfO_2	1.000	I			
E0003772	ZrO_2	91.93 wt%	B	—		G. A. Zhorov
	CaO	5.800	S			
	TiO_2	1.000	I			
E0003773	ZrO_2	91.93 wt%	B	1900.		G. A. Zhorov
	CaO	5.800	S			
	TiO_2	1.000	I			
E0003774	ZrO_2	91.93 wt%	B	2330.		G. A. Zhorov
	CaO	5.800	S			
	TiO_2	1.000	I			
E0003775	ZrO_2	83.41 wt%	B	1125.	Air	G. A. Zhorov
	SiO_2	11.20	S			
	Na_2O	5.100	I			
E0003776	ZrO_2	66.00 wt%		—		G. A. Zhorov
	SiO_2	33.15				
	Al_2O_3	1.600				
E0003777	ZrO_2	66.01 wt%		1800.		G. A. Zhorov
	SiO_2	33.15				
	Al_2O_3	1.600				
E0003778	ZrO_2	66.00 wt%		2060.		G. A. Zhorov
	SiO_2	33.15				
	Al_2O_3	1.600				
E0003779	ZrO_2	82.30 wt%	B	—		G. A. Zhorov
	SiO_2	10.00	S			
	CaO	6.900	S			
E0003780	ZrO_2	82.30 wt%	B	2330.		G. A. Zhorov
	SiO_2	10.00	S			
	CaO	6.900	S			
E0003785	ZrO_2	91.14 wt%		—		V. Zapechnikov
	CaO	6.000				
	SiO_2	0.9000				
E0003786	ZrO_2	89.60 wt%		—		V. Zapechnikov
	CaO	7.950				
	SiO_2	0.3600				

Table III. *(Continued)*

EKEY	CCOM	CCOMA		D	TRTEM	TRATM	AU
E0003787	ZrO_2	97.35	wt%		—		G. A. Zhorov
	TiO_2	1.150					
	CaO	0.9500					
E0003788	ZrO_2	97.35	wt%		1666.		G. A. Zhorov
	TiO_2	1.150					
	CaO	0.9500					
E0003789	ZrO_2	97.35	wt%		1844.		G. A. Zhorov
	TiO_2	1.150					
	CaO	0.9500					
E0003790	ZrO_2	97.35	wt%		2351.		G. A. Zhorov
	TiO_2	1.150					
	CaO	0.9500					
E0003791	ZrO_2	91.92	wt%		—		G. A. Zhorov
	TiO_2	1.000					
	CaO	5.800					
E0003792	ZrO_2	91.92	wt%		—		G. A. Zhorov
	TiO_2	1.000					
	CaO	5.800					
E0003793	ZrO_2	91.92	wt%		1902.		G. A. Zhorov
	TiO_2	1.000					
	CaO	5.800					
E0003794	ZrO_2	91.92	wt%		2323.		G. A. Zhorov
	TiO_2	1.000					
	CaO	5.800					
E0003795	ZrO_2	1.000	M		—		M. E. Whitson, Jr.
E9000216	ZrO_2	94.00	wt%	B	—		G. Neuer
	CaO	6.000		S			
E9000217	ZrO_2	94.00	wt%	B	1000.	Vacuum	G. Neuer
	CaO	6.000		S			
E9000218	ZrO_2	94.00	wt%	B	1600.	Vacuum	G. Neuer
	CaO	6.000		S			
E9000219	ZrO_2	94.00	wt%	B	1300.	Vacuum	G. Neuer
	CaO	6.000		S			
E9000220	ZrO_2	94.00	wt%	B	1900.	Vacuum	G. Neuer
	CaO	6.000		S			
E9000221	ZrO_2	94.00	wt%	B	1900.	Vacuum	G. Neuer
	CaO	6.000		S			

Signification of all descriptor codes

EKEY	Key
CCOM	Symbol of component
CCOMA	Amount
CCOMD	Supplementary code
TRTEM	Thermal treatment: temperature
TRATM	Thermal treatment: atmosphere
AU	Author(s)

Units of descriptors

TRTEM	[K]

signification of codes

B	Balance
I	Impurity
S	Stabilizer

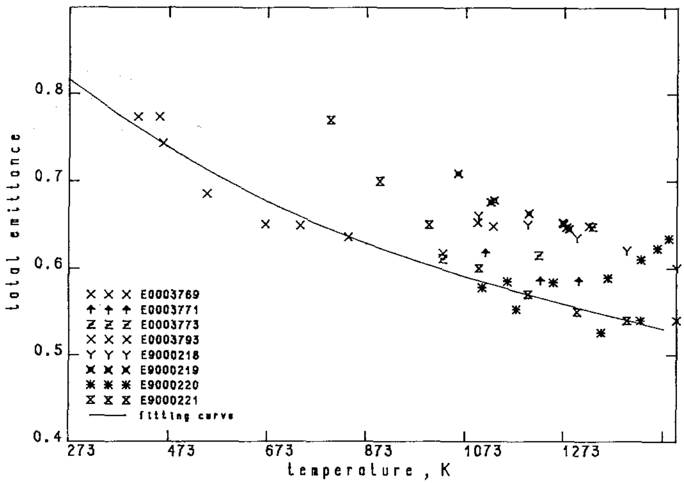

Fig. 3. Total emittance of ZrO_2. The number of curves, plotted in Fig. 1, is reduced by limiting the descriptors. Treatment temperature, between 1000 and 2000 K; chemical composition, $ZrO_2 > 90$ wt% and $CaO < 5$ wt%.

content and that the samples were partly annealed at temperatures above 2000 K and partly untreated. By restraining the measurement values to sample with

- a composition of $ZrO_2 > 90$ wt% and
- an annealing temperature of $1000 < T < 2000$ K,

the range of scatter becomes considerably smaller as shown in Fig. 3, where the remaining curves are plotted together with a fitting curve.

6. CONCLUSIONS

A great number of information items describing a relation among measured properties, measurement technique, and material characterization can be stored in THERSYST. The collection of all these data is very time-consuming. As long as the measurement results are presented in a form which does not permit quick and precise extraction of the data, it cannot be performed economically. Two steps are necessary to improve the input of thermophysical data into a data base with reference to quality, completeness, and rationalization.

(1) An international agreement should be reached for a more or less standardized form of data presentation. An essential advantage

also for the producer of data who presents his results in a clearly arranged form is that the information is transferred into a data base without any mistake or omission.

(2) An international cooperation should be strived for, with the aim that data are collected at institutions distributed worldwide, taking into account the following two very important conditions. (a) Double work by storing data from identical sources at two places should be prevented. (b) The structure of the stored data should have such a form that a data exchange between these institutions is possible without problems.

As a model, cooperation is planned in this field among several institutions of the German Working Group on Thermophysical Properties (Arbeitskreis Thermophysik der Deutschen Keramischen Gesellschaft).

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REFERENCES

1. J. H. Westbrook, H. Behrens, G. Dathe, and S. Iwata (eds.). *Materials Data Systems for Engineering* (Fachinformationszentrum Energie, Physik, Mathematik, Karlsruhe, 1986).
2. H. H. Li and C. Y. Ho, in *An On-Line Materials Property Data Base*, Publ. MPC-20, J. A. Graham, ed. (Am. Soc. Mech. Eng., New York, 1983), pp. 107–119.
3. T. Araki, T. Baba, and A. Ono, in *Proceedings of the 1st Asian Thermophysical Properties Conference* (China Academic, Beijing, 1986).
4. R. Brandt, K. Löffler, G. Jaroma-Weiland, G. Neuer, and G. Pflugfelder, *THERSYST, a Database with Program System for Thermophysical Properties*, Rep. No. 5-229 (Institut für Kernenergetik und Energiesysteme, University of Stuttgart, 1987).
5. R. Rühle, *Atomkernenergie (ATKE)* **26**:188 (1975).
6. B. Wörner and G. Neuer, *High Temp. High Press.* **11**:383 (1979).
7. K. D. Maglić, A. Cezairliyan, and V. E. Peletsky (eds.), *Compendium of Thermophysical Property Measurement Methods, Vol. 1. Survey of Measurement Techniques* (Plenum Press, New York, 1984).
8. G. A. Zhorov and R. M. Zakharov, *High Temp.* **18**:578 (1980).

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