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A PC Program to Standardize the Description of Measurement Results of Thermophysical Properties of Solids[1]

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One of the most serious problems of factual databases is the data input, especially when the relation between the properties of interest and the material or experimental parameters is complex. In order to enable data input in the field of thermophysical properties, a new special PC program has been developed, which facilitates the data input by means of a windows technique. In these windows, the user is presented with input fields where alphanumerical values or integers can be inserted corresponding to a given list of descriptors. In principle, this list can be extended by each user. The problem, however, is then to keep all other users informed about the updated list of descriptors. It is intended to establish a community of users of this programme for the purposes of standardization of data input and acceleration of information exchange about measurement results.

KEY WORDS: database; input program; thermophysical properties.

1. INTRODUCTION

At the tenth Symposium on Thermophysical Properties the database THERSYST was presented for the first time to the community of thermophysical properties [1]. Since then, progress has been made both with respect to the number of stored data and to the improvement of the applicability by other users.

Unlike other material databanks like POLYMAT [2] and ALUSELECT [3], THERSYST takes into account the dependence of thermophysical properties on a large number of material parameters, and

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the given information can be traced back to the original source [1]. All available data from the literature or from measurement laboratories are stored after checking the reliability. A pool of data sets can be made available in order to intercompare these sets, to establish relations between a thermophysical property and certain material parameters, or to elaborate recommendations for users' materials about the most probable values of the properties. Examples of such applications are the evaluation of the literature data for the thermal conductivity of thermal barrier coatings [4] or the determination of the dependence of the emissivity of steel on surface roughness [5].

There exist some efforts to introduce electronic publishing of experimental results additonal to the usual, written papers. For that purpose CODATA (Committee on Data for Science and Technology) has established a new task group, called EXPERIDAT (Database for Experimental Data and Telepublishing). One intention of this group is to convince publishers of corresponding scientific papers that no paper should be accepted without an additional description of the data in a form which can be more or less directly used as an input into a database. The most important prerequisite for that purpose is the availability of an internationally accepted form of presentation. This paper is a contribution to find an international agreement for such a standardization in the domain of thermophysical experiments.

2. DESCRIPTION OF INPUT PROGRAM

It is well-known that the thermophysical properties of solid materials depend on material parameters (chemical composition, microstructure, etc.) and experimental conditions. In a factual database the information of all factors of influence should be stored and the original context between the property data and the describing data should be preserved. In THERSYST this problem was solved by using a class concept. The relevant information is converted into a standardized form given by the scheme of category and is stored in the form of a data set. The scheme of category is divided into five classes.

Class 1: Material designation and typical constants.

Class 2: Characterization of specimen to be studied.

Class 3: Experiment description.

Class 4: Description of the thermophysical property and the property data.

Class 5: Bibliographic information on literature source.

```
class: MATCHAR.2

structure: POLC (*)  Crystal Str: (CUB)(*)  Solid Solution:    (*)
microstructure:
lattice parameter: 5.6787A; grain size: 12 micro-meter


preparation:  CAST   HOMO        (*)
sample treatment - preparation
  mechanical:  POLI         (*)
  chemical:    CHET         (*)
  thermal: AGED (*)       temperature:  430.00 [ 11]   time:      2.000 [582]
                          atmosphere:  air
                          pressure:    1         [569]  field:            [650]
  kind of irradiation:     (*)dose:              [600]  temp:             [ 10]
  further treatments:      (*)
    INPUT CORRECT (Y/N)     N

  ADD NEW DATA TO EXISTING DATA
```

Fig. 1. Input window for the material characterization (class 2).

In each class the information is stored by descriptors which are in a numerical or coded form. It guarantees the proper operation of retrieval in the database because each descriptor can be used as a search criterion. Textual descriptors are also available for supplementary information, which cannot be classified. The structure and the content of THERSYST are described in detail in Refs. 1 and 6.

For the input of the describing data a special PC program has been developed. It operates by means of a window technique. Classes 1, 3, 4, and 5 use one input window each; for class 2, three windows are necessary. Figure 1 shows one of the input windows for class 2 (material characteriza-

```
class: MATCHAR.2       
                         TRCL triclinic
structure: POLC (*)  Cr  MONO monoclinic (simple)
microstructure:          MOBA monoclinic (base centered)
lattice parameter: 5.67  ORTH orthorhombic (simple)
                         ORBA orthorhombic (base centered)
                         ORBO orthorhombic (body centered)
                         ORFA orthorhombic (face centered)
preparation:  CAST   HO  TETR tetragonal (simple)
sample treatment - prep  TEBO tetragonal (body centered)
  mechanical:  POLI      (CUB) cubic (simple)
  chemical:    CHET      BCC  cubic (body centered)
  thermal: AGED (*)      FCC  cubic (face centered)            00 [582]
                         HEX  hexagonal
                         HCP  hexagonal (close-packed)               [650]
  kind of irradiation:   TRG  trigonal                               [ 10]
  further treatments:    RHOM rhombohedral
    INPUT CORRECT (Y/N)  SCHE scheelite
                         ANFL antifluorite
                         NACL rocksalt           (NaCl)
  ADD NEW DATA TO EXISTING DATA
```

Fig. 2. The same window as Fig. 1, however, with additionally displayed codes for the descriptor "crystal structure."

```
class:EIGENSCH        modus:                          DocuNr.: J0002345
key:    860033 (*)                                               SNAM :AMAL
property:  EMI        (*) [220]    specification:       (*)     M-key: 860056
measuring direction:                                            N-key: 860036
                                                                E-key: 860033
specification of radiative properties:
   spectral range: (TOT) (*) wavelength:   0.600 [520]    12.600 [520]
   geometric relations: HEMI (*) angle of incidence      /emergence      [deg
   polarization:           (*)
specification of electrical resistivity: AC-frequency:                   [Hz
spec. of thermal expansion:  ref. temp.:   298.00[K]  ref. value:        [510

variable:   T        (*)  [ 10]         measuring temperature:           [ 10
parameter: RF    (*)     (*)      (*)      (*)
accuracy:  5.00 %  classif.:SMOO(*) BitPat-uncert:2.3e-5   A valuation:    (*
number of data sets:   1
data-set-No.:      3456    tab/fig-No.: fig.1     column/line/curve-No:3
remark:N                INPUT CORRECT (Y/N)       N
```

```
ADD NEW DATA TO EXISTING DATA
```

Fig. 3. Input window for the property description (class 5).

tion) and Fig. 3 shows the window for class 5 (property description). An asterisk indicates the fields in which a code should be typed. If a cursor is placed at such a field, by pressing the F10-key the selection window is opened and the pop-up window displays the possible inputs for this field. In class 2 the cursor was placed on the field "crystal structure"; in class 5, on the field "spectral range." In the pop-up window the codes for each descriptor are listed (Figs. 2 and 4). The selected input is transferred automatically. The same procedure is used for unit codes. These fields normally have default values which are coded in SI-units. The list of codes can

```
class:EIGENSCH        mo
key:    860033 (*)       SOL   solar                                 :AMAL
property:  EMI        (* SPEB  spectral band: cut-on/cut-off        y: 860056
measuring direction:     SPEL  spectral line: center waveleng       y: 860036
                         SPEX  spectral: wavelength is a vari       y: 860033
specification of radiat (TOT)  total
   spectral range:  TOT                                             0]
   geometric relations: HEMI (*) angle of incidence      /emergence      [deg
   polarization:           (*)
specification of electrical resistivity: AC-frequency:                   [Hz
spec. of thermal expansion:  ref. temp.:   298.00[K]  ref. value:        [510

variable:   T        (*)  [ 10]         measuring temperature:           [ 10
parameter: RF    (*)     (*)      (*)      (*)
accuracy:  5.00 %  classif.:SMOO(*) BitPat-uncert:2.3e-5   A valuation:    (*
number of data sets:   1
data-set-No.:      3456    tab/fig-No.: fig.1     column/line/curve-No:3
remark:N                INPUT CORRECT (Y/N)       N
```

```
ADD NEW DATA TO EXISTING DATA
```

Fig. 4. The same window as Fig. 3, however, with additionally displayed codes for the descriptor "spectral range."

be extended by each program user. In principle, also, the list of descriptors in each class can be enlarged but it should be made by the data bank producer only.

The described input program inserts the data into a dBase databank. From this database the data are exported together with measured property data by means of ASCII-files either to THERSYST installed on the VAX mainframe or into PC-THERSYST.

3. ACTUAL STATE OF THE THERSYST DATA INPUT

At present THERSYST is installed at four German institutes and in each of them thermophysical data are stored for selected group of materials.

IKE:[4] Metallic elements and alloys, some specific composites.

ITU:[5] Actinide, transuranium elements, and their compounds.

IMF:[6] Ceramics.

PI:[7] Heat insulation materials.

The data collection on IKE contains about 6000 data sets on 10 thermophysical properties of 850 metallic materials. The literature published in the period from 1960 up to now has been evaluated. In the case of light-metal alloys the experimental data measured since 1920 were also included. Furthermore, 1500 data sets on ceramics and 300 on selected composites such as C/SiC, SiC/SiC, or metal matrix composites with light metal matrix have been stored. At ITU above 1500 data sets have been stored primary on actinide oxides and carbides. The input of data on transuranium elements and alloys is continued. At PI the data input on foil-spacer and insulants for high-temperature application has been started.

4. INTERNATIONAL COOPERATION

As described in Section 2 there is now available a computer program for an easy and convenient data input on PC. The system to describe the measurement and the material is a result of numerous discussions of experts working in the field of thermophysical properties. However, this system is not rigid: it can be enlarged, and new descriptions can be added.

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[7] Physikalisches Institut der Universität Würzburg: Dr. O. Nielsen.

The best way to do this is improving by using: as many experiments as possible should put their data—after these are ready for publishing!—via this PC program into the THERSYST database. All participants in such an International Thermophysical Properties Data Base Club submitting their own or new literature data are entitled to getting data of interest from the pool. The suggestions to modify the description system, coming from the participants, will be taken into consideration and implemented into the program. Updates will be sent regularly to all users because only a uniform input program can guarantee that the data fit together in the database. By actively making use of this data exchange we will achieve an internationally standardization of data input for thermophysical database.

5. CONCLUSIONS

THERSYST has been proven to work. A large number of thermophysical data have been accumulated. This is the right time to introduce THERSYST for worldwide use. The proposed user club could be a first step toward a new age of data publishing, but first of all it offers a new kind of communication between measurement laboratories. The program is available free of a charge and those interested in this cooperation are requested to contact one of the authors of this paper.

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