International Journal of Thermophysics, Vol. 7, No. 4, 1986

Computerized Comprehensive Numerical Data System on the Thermophysical and Other Properties of Materials Established at CINDAS/Purdue University[1]

C. Y. Ho[2] and H. H. Li[2]

A computerized materials properties numerical data system has been developed and established at the Center for Information and Numerical Data Analysis and Synthesis (CINDAS) of Purdue University, which is a comprehensive, one-line, interactive, menu-driven, user-friendly, expert data system. This data system contains both critically evaluated reliable reference data and experimental data on the thermophysical, mechanical, electrical, optical, and other properties of various types of materials. It permits both the search of data and information for specified materials and properties and the search for materials that meet a set of requirements specified by the user (i.e., computer-aided materials selection). It permits also the on-line functional manipulation, statistical analysis, and mthemtical study of the retrieved data. The development, operation, functions, scope, contents, and other features of the data system are presented and discussed.

KEY WORDS: computerized numerical data system; electrical properties, materials properties data system; mechanical properties; numerical data base; optical properties; thermophysical properties.

1. INTRODUCTION

The Center for Information and Numerical Data Analysis and Synthesis (CINDAS) of Purdue University has been compiling and evaluating materials properties data since 1957 and has been developing a *computerized* materials properties data system since 1972. In earlier years the data system development had been for a few properties of a few thousand

[1] Paper presented at the Ninth Symposium on Thermophysical Properties, June 24–27, 1985, Boulder, Colorado, U.S.A.

[2] Center for Information and Numerical Data Analysis and Synthesis (CINDAS), Purdue University, West Lafayette, Indiana 47906, U.S.A.

0195-928X/86/0700-0949$05.00/0

materials, including elements, fluids, alloys, compounds, ceramics, polymers, etc. In recent years the development has been concentrated on several large groups of materials such as dielectric materials, composite materials, aerospace structural alloys, infrared detector/sensor materials, etc., and the number of properties covered is very large. This has resulted in a comprehensive materials properties data system. This data system is being updated continuously and expanded rapidly.

The necessity for and the advantages of the establishment of a computerized comprehensive data system on materials properties are obvious. First of all, as the existing data and information on materials properties are widely scattered and buried in the vast and diverse worldwide scientific and technical literature, engineers, scientists, and designers are unfortunately using but a small fraction of them. The establishment of the comprehensive materials properties data system will provide a remedy to this disturbing situation.

This disturbing situation, of course, has led also to the establishment of the many bibliographic information retrieval systems currently prevailing. However, the usefulness of bibliographic information retrieval systems is limited because they do not provide explicit actual data but give only potential sources of data, and engineers and scientists really want data, not documents. After receiving a list of bibliographic citations from a bibliographic retrieval system, the inquirer must take the time to acquire the documents (and often find that many are unavailable), read them (and often find that most of them are irrelevant), and extract the pertinent data and information from the remaining relevant documents (and often find that different documents give different answers, if any). Therefore, even if the documents acquired by the inquirer seem relevant, the procedure gives no assurance that the data and information obtained are reliable and usable.

Consequently, as the material property data recorded in the scientific and technical literature are often conflicting, widely diverging, and subject to large uncertainty, the experimental data must be critically evaluated and analyzed to generate reliable reference data. The availability of both the critically evaluated reference data and the raw experimental data from the comprehensive data system at CINDAS is one of its many distinguished features.

The potential advantages of the computerized comprehensive materials properties data system established at CINDAS are listed in Table I. It is an on-line, interactive, menu-driven, user-friendly, expert data system for on-line ready access and instant retrieval and dissemination of data and information directly to the fingertips of enginers, scientists, and designers through computer terminals across the nation. This data system

Table I. Potential Advantages of the Computerized Comprehensive Materials Properties Data System Established at CINDAS/Purdue University

(1)	Providing the user a single source for comprehensive data and information
(2)	Allowing computer-aided materials selection (CAMS)
(3)	Instant on-line retrieval, display, functional manipulation, statistical analysis, and mathematical study of data
(4)	Constant updating of data and information
(5)	Easy comparison of data
(6)	Easy conversion of units
(7)	Graphical and tabular display options
(8)	Integration with design algorithms and with CAD-CAM programs
(9)	Ascertaining equivalency of different materials
(10)	Increased awareness of the topography of the state of knowledge and of the inconsistencies, gaps, and voids in the data
(11)	Increased awareness of potential better choices other than traditional materials in design
(12)	Improvement of both the scope and the effectiveness of collecting, processing, storing, accessing, retrieving, disseminating, and applying data and information
(13)	Ensuring timely and effective exchange and transfer of data and information
(14)	Ensuring the elimination of unnecessary wasteful duplication of efforts and resources
(15)	Increasing the productivity and cost effectiveness of research, development, engineering, or studies programs that require data and information
(16)	Closing the time gap between research and application
(17)	Reducing design cycles
(18)	Providing R&D funding entities with state-of-the-art information for program planning

will certainly help to ensure that the past, current, and future R&D results on materials properties be well organized and highly visible, directly usable, readily available, easily accessible, and instantly retrievable.

2. DATA SYSTEM DEVELOPMENT

The computerized materials properties data system contains a number of data bases and each data base is on a group of materials.

The development of each data base involves

(i) the in-depth cognizance and acquisition of the relevant worldwide scientific and technical literature;

(ii) the exhaustive extraction and compilation of experimental data from the acquired pertinent research documents;

(iii) the critical evaluation, analysis, correlation, and synthesis of the compiled raw experimental data to generate reliable reference data;

(iv) the computerization of both the raw experimental data and the CINDAS-generated reliable reference data to create various data files;

(v) the integration of the various data files to establish an operational computeratized data base; and

(vi) the operation, maintenance, and continuing update and expansion of the established data base.

The data system enables the on-line interactive retrieval of

(i) data and information in tabular and graphical forms for specified materials, properties, information items, independent variables, parameters, etc.., and

(ii) a list of candidate materials that meet a set of requirements specified by the user (i.e., computer-aided materials selection)

and enables also the on-line functional manipulation, statistical analysis, and mathematical study of the retrieved data. The input numerical data are all in standard units, but the output data can be in any system of units as selected by the user.

This data system has been developed to be truly a computerized, comprehensive, on-line, interactive, menu-driven, user-friendly, intelligent data system. It is so user-friendly and intelligent that the user can easily search, retrieve, and manipulate the data from the data system without knowing anything about the computer, without reading any lengthy user manual, without attending any user training workshop, and without knowing any query language, any set of special commands, any standardized names of materials, properties, variables, parameters, or the correct spelling of any of the names.

In the extraction and compilation of the experimental data, since numerical property data are meaningful and useful only if adequate information on the test material and on the property measurement is also provided, CINDAS has always paid special attention to extract such information from the research document together with the numerical data. Thus, each set of data extracted and compiled by CINDAS consists of numerical data points (as a function of temperature or other independent variable) and pertinent information on the specification and characterization of the test material and on the method and conditions of the property measurement, such as composition, purity, density, porosity, microstructure, material construction configuration, material processing, sample preparation, geometry and dimensions, surface condition, material history, manufacturer, heat treatment, cold working, method of

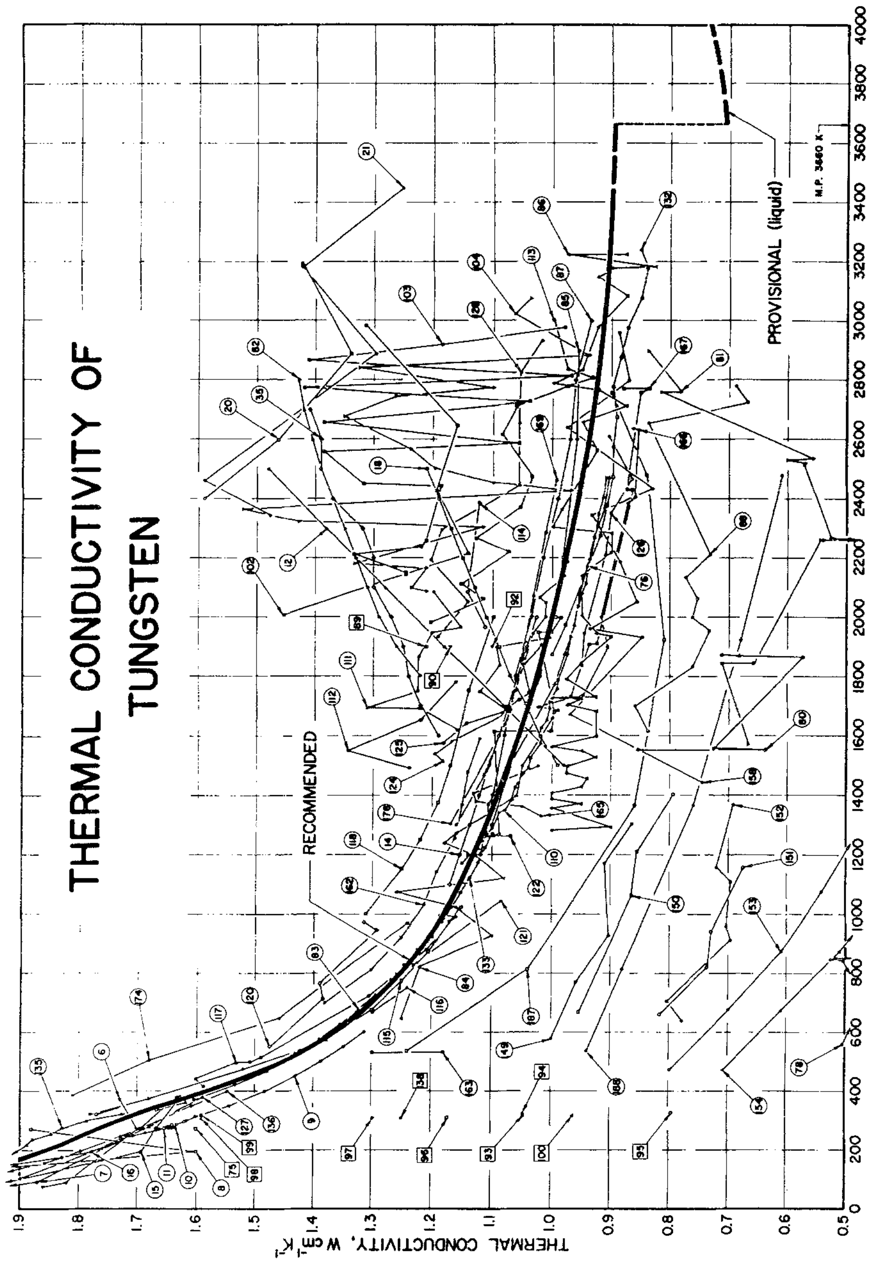

Fig. 1. An examples of CINDAS' result of data evaluation and analysis.

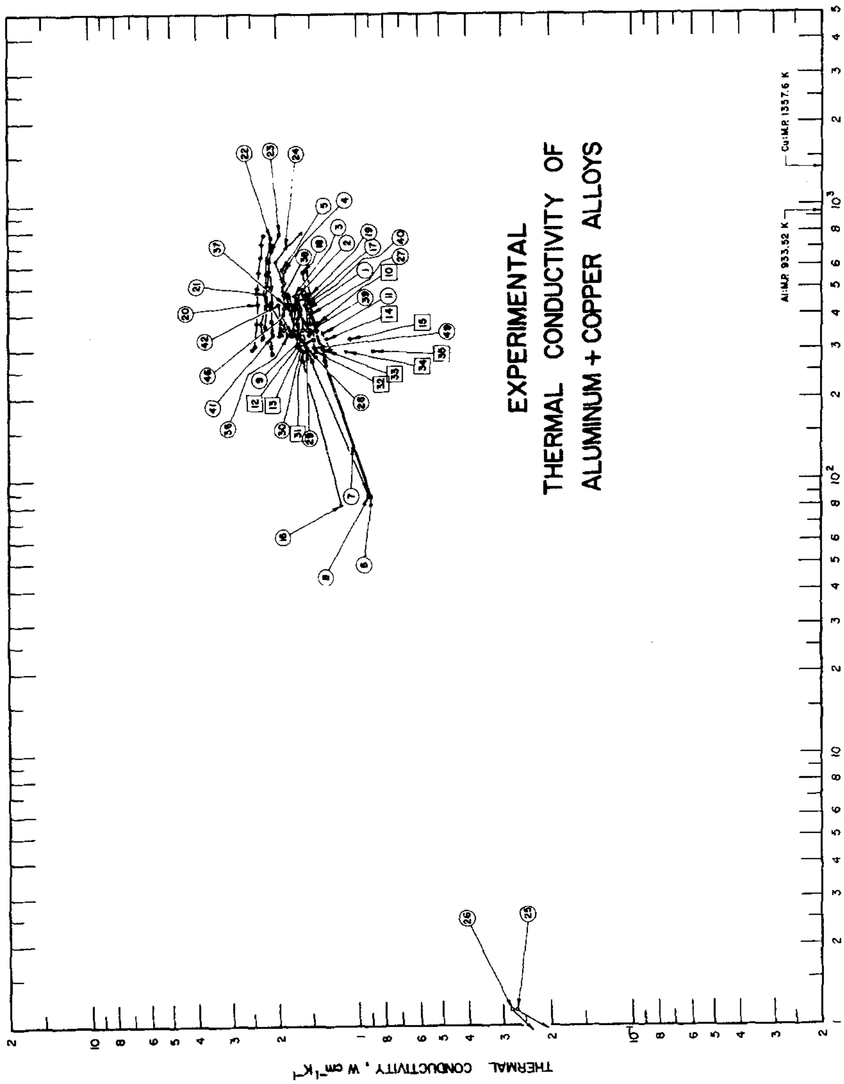

Fig. 2. An example of experimental data used in CINDAS' data synthesis.

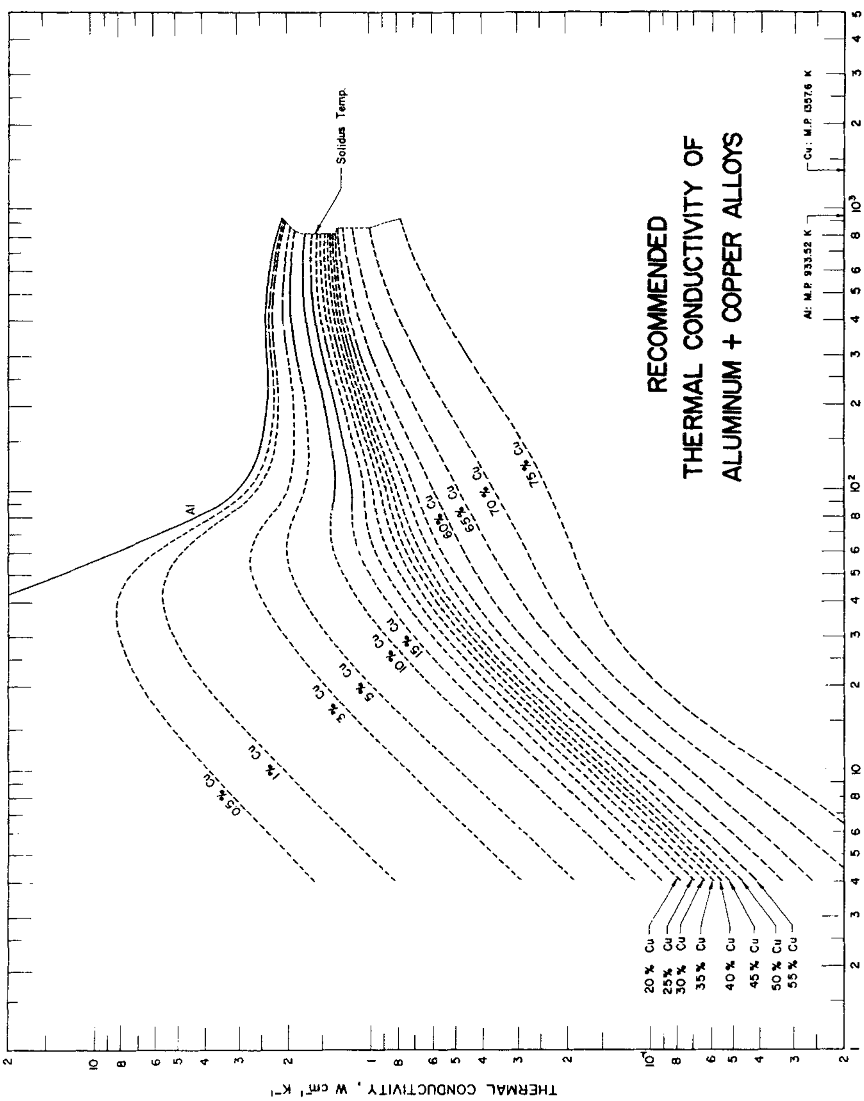

Fig. 3. An example of CINDAS' result on data synthesis (based on experimental data shown in Fig. 2.).

measurement, test environment, heat flow direction, heating rate, heat-up time, heat-up temperature, holding time at temperature, cooling rate, type of heat source, loading rate, applied magnetic field intensity, etc., insofar as these are contained in the original document.

In the critical evaluation, analysis, correlation, and synthesis of the experimental data, CINDAS' long-established methodology has been followed, which has been discussed in detail elsewhere [1]. Figure 1 shows an example of CINDAS' result of data evaluation and analysis [2] and the combination of Figs. 2 and 3 shows an example of the result of data synthesis [3].

3. SCOPE AND CONTENTS OF THE DATA SYSTEM

This data system contains the data and information on the properties of various types of materials which are stored in different data bases. Some data bases are not to be opened to the public for on-line access. Others such as the data base on dielectric materials developed for and sponored by the Electric Power Research Intitute are to be opened to the public for on-line access in due course.

These data bases are comprehensive in the sense that they cover a large number of properties and materials. For instance, the data base on dielectric materials covers more than 100 properties of several hundred materials and is continuously being expanded and updated so that it will eventually contain all the available reliable data and information on all important electrical insulating liquids, gases, solids, and combinations

Table II. Categories of Data and Information Covered in the Data Base on Dielectric Materials

(1)	Thermal properties
(2)	Electrical properties
(3)	Physical properties
(4)	Chemical properties
(5)	Optical and thermoradiative properties
(6)	Mechanical properties
(7)	Flammability properties and information
(8)	Health hazard and environmental impact information
(9)	Processability and manufacturing information
(10)	Material characteristics and specification
(11)	Aging, degradation, erosion, and corrosion information
(12)	Usefulness and application information
(13)	Producer, supplier, availability, and cost range

Table III. Mechanical Properties Covered in the Computerized Data Base on Aerospace Structural Composites and Metals

(1)	Compressive creep strain
(2)	Compressive creep strength
(3)	Compressive modulus, E(C, X)
(4)	Compressive modulus, E(C, Y)
(5)	Compressive modulus, E(C, Z)
(6)	Compressive modulus, E(C, 11)
(7)	Compressive modulus, E(C, 22)
(8)	Compressive modulus, E(C, 33)
(9)	Compressive strain
(10)	Compressive strain at fracture
(11)	Compressive strength, ultimate, *F*(*C*, *U*)
(12)	Compressive strength, yield, *F*(*C*, *Y*)
(13)	Compressive stress
(14)	Compressive Young's modulus, *E*(*C*)
(15)	Crack strength, yield
(16)	Critical stress intensity, plane-stress, *K*(*C*)
(17)	Elastic constant, *C*(11)
(18)	Elastic constant, *C*(12)
(19)	Elastic constant, *C*(13)
(20)	Elastic constant, *C*(22)
(21)	Elastic constant, *C*(23)
(22)	Elastic constant, *C*(33)
(23)	Elastic constant, *C*(44)
(24)	Elastic constant, *C*(55)
(25)	Elastic constant, *C*(66)
(26)	Elongation
(27)	Energy-release rate, *G*(IC)
(28)	Energy-release rate, *G*(IIC)
(29)	Flexural modulus
(30)	Flexural strength
(31)	Flexural strength, yield
(32)	Flow stress, compressive
(33)	Flow stress, tensile
(34)	Fracture surface work, interlaminar
(35)	Fracture toughness, plane-strain, *K*(IC)
(36)	Critical fracture toughness, *K*(*C*)
(37)	Hardness, Brinell (BHN)

Table III *(Continued)*

(38)	Hardness, Rockwell
(39)	Hardness, Vickers (DPH or DPN)
(40)	Impact energy, Charpy keyhole notch
(41)	Impact energy, Charpy V-notch
(42)	Impact energy, Izod V-notch
(43)	Impact strength (impact energy)
(44)	In-plane shear modulus
(45)	In-plane shear strength
(46)	Interfacial shear strength
(47)	Interlaminar shear strength, ILSS
(48)	Isochronous rupture strength
(49)	Maximum fatigue strain
(50)	Modulus of rigidity
(51)	Modulus of rupture, torsional
(52)	Notch strength, tensile
(53)	Notch strength, tensile, normalized
(54)	Poisson's ratio, compressive, $NU(C, XY)$
(55)	Poisson's ratio, compressive, $NU(C, YX)$
(56)	Poisson's ratio, compressive, $NU(C, 12)$
(57)	Poisson's ratio, compressive, $NU(C, 13)$
(58)	Poisson's ratio, compressive, $NU(C, 21)$
(59)	Poisson's ratio, compressive, $NU(C, 23)$
(60)	Poisson's ratio, compressive, $NU(C, 31)$
(61)	Poisson's ratio, compressive, $NU(C, 32)$
(62)	Poisson's ratio, tensile, $NU(T, XY)$
(63)	Poisson's ratio, tensile, $NU(T, YX)$
(64)	Poisson's ratio, tensile, $NU(T, 12)$
(65)	Poisson's ratio, tensile, $NU(T, 13)$
(66)	Poisson's ratio, tensile, $NU(T, 21)$
(67)	Poisson's ratio, tensile, $NU(T, 23)$
(68)	Poisson's ratio, tensile, $NU(T, 31)$
(69)	Poisson's ratio, tensile, $NU(T, 32)$
(70)	Rail shear modulus
(71)	Rail shear strength
(72)	Reduction in area

Table III *(Continued)*

(73)	Residual strain
(74)	Residual strength, compressive
(75)	Residual strength, compressive, yield
(76)	Residual strength, short-beam shear
(77)	Residual strength, tensile
(78)	Residual strength, tensile, yield
(79)	Rupture stress
(80)	Shear modulus, $G(XY)$
(81)	Shear modulus, $G(12)$
(82)	Shear modulus, $G(13)$
(83)	Shear modulus, $G(23)$
(84)	Shear modulus, $G(32)$
(85)	Shear strain
(86)	Shear strain at fracture
(87)	Shear strength, ultimate
(88)	Shear strength, yield
(89)	Shear stress
(90)	Short-beam shear strength
(91)	Tensile creep strain
(92)	Tensile creep strength
(93)	Tensile modulus, $E(T, X)$
(94)	Tensile modulus, $E(T, Y)$
(95)	Tensile modulus, $E(T, Z)$
(96)	Tensile modulus, $E(T, 11)$
(97)	Tensile modulus, $E(T, 22)$
(98)	Tensile modulus, $E(T, 33)$
(99)	Tensile strain
(100)	Tensile strain at fracture
(101)	Tensile strength, ultimate, $F(T, U)$
(102)	Tensile strength, yield, $F(T, Y)$
(103)	Tensile stress
(104)	Tensile Young's modulus, $E(T)$
(105)	True nonelastic strain at max load
(106)	True strain
(107)	True stress

Table IV. Example of One Set of Data on Thermal Expansion in the Data Base on Aerospace Structural Composites

Material: Hercules AS/Hercules 3501-6 Date set 1

Property: Thermal expansion

Composition:

65.0	Weight percent	Hercules AS-1 graphite
35.0	Weight percent	Hercules 3501-6 epoxy

Supplier/manufacturer: Prepreg tapes from commercial source

Composite material layup:

Fiber reinforcement: 2D (0)

Number of plies: 5

Processing of Composite materials:

Rigidization method (prepreg):

Prepreg tape cut to size and 5 plies layed up by hand to proper dimensions of $12 \times 24 \times 0.025$ in. on release agent-coated stainless-steel plate; on the top were placed, in order, a layer of release cloth, a layer of open-cell foam/random-fiber bleeder cloth, and a layer of polyethylene film; whole unit was placed in blanket press and cured.

Curing/densification sequence:

Cured at 100°C for 1 h and for 3 h at 177°C

Additional prparation/conditioning prior to masurement

Environment: Moisture

descriptions—Textual

Moisture conditioned to 1.69% ave. moisture content.

Speciment idntification:

Dimensions (geometry):

Length, 57.2 mm

Width, 6.35 mm

Orientation with respect to material: Interlaminar, through thickness

Measurement method for property Y:

Name/description:

Daytronic model DS200 LUDT combined with quartz dilatometer

Measured properties:

X: Temperature, K

Y: Thermal expansion, percent

Table IV. *(Continued)*

Data points:

X	Y	Remark:
2.080E+02	−1.810E−01	
2.305E+02	−1.350E−01	
2.673E+02	−6.990E−02	
2.867E+02	−3.110E−02	
3.134E+02	3.040E−02	
3.377E+02	7.380E−02	
3.637E+01	1.420E−01	
2.086E+02	−1.900E−01	
2.305E+02	−1.420E−02	
2.673E+02	−8.960E−02	
2.861E+02	−3.490E−02	
3.140E+02	3.650E−02	
3.376E+02	1.000E−01	
3.643E+02	1.590E−01	
2.080E+02	−1.740E−01	
2.299E+02	−1.320E−01	
2.673E+02	−8.050E−02	
2.867E+02	−2.960E−02	
2.980E+02	−7.000E−04	
3.140E+02	4.260E−02	
3.377E+02	8.900E−02	
3.643E+02	1.510E−01	
1.949E+02	−1.990E−01	Smooth values
2.329E+2	−1.410E−01	
2.714E+02	−7.210E−02	
3.098E+02	1.450E−02	
3.442E+02	9.960E−02	
3.673E+02	1.630E−01	

Data—Comments:

Ave. moisture content 1.69%

TLE (percent) = −6.745E−02 + 2.047E−03T + 4.546E−08T[2] for 1.87% ave. moisture content (TLE, thermal linear expansion)

Reference

Moisture and thermal expansion of composite materials

Cairns, D. S., Adams, D. F.

Wyoming Univ., Dept. Mech. Eng., Laramie, 210 pp., 1981

(AD-A109 131, UWME-DR-101-104-1, ARO-16370.5-MS) thereof. If provides also commercial and applications data in addition to technical data. The 13 categories of data and information covered in the data base on dielectric materials, for example, are listed in Table II.

One of the data bases is on the aerospace structural composites and metals sponsored by the Department of Defense. This data base contains data and information on 17 thermophysical properties and 40 mechanical properties. However, since composite materials are highly anisotropic and structural dependent, in order to identify fully the data exactly with the property to which they belong, each property must be defined extremely precise. As a result, many of the properties are each subdivided into several subproperties. For example, the mechanical properties covered in this comprehensive data base have been subdivided into 107 subproperties as listed in Table III.

As an example to show the data and information stored in this data base, Table IV contains one set of data on the thermal linear expansion of a particular sample of Hercules AS/Hercules 3501-6 graphite/epoxy composite. The pertinent information on this particular sample and on the measurement is given in the table. It should be noted again that all the thousands of data sets in the data base can be pinpointed for computer retrieval.

REFERENCES

1. C. Y. Ho and Y. S. Touloukian, in *Proceedings of the Eighth Symposium on Thermophysical Properties, Vol. II* (ASME, New York, 1982), pp. 419–430.
2. C. Y. Ho, R. W. Powell, and P. E. Liley, *J. Phys. Chem. Ref. Data* **3** (Suppl. 1):692 (1974).
3. C. Y. Ho, M. W. Ackerman, K. W. Wu, S. G. Oh, and T. N. Havill, *J. Phys. Chem. Ref. Data* 7:959 (1978).