Numerical Databases on Materials Property Data at CINDAS/Purdue University

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Computerized numerical databases on the thermophysical, thermoradiative, mechanical, electronic, optical, and other properties of various classes of technologically important materials such as metals, alloys, composites, polymers, dielectric materials, detector/sensor materials, microelectronics packaging materials, inorganic and organic fluids, and refrigerants have been developed by the Center for Information and Numerical Data Analysis and Synthesis (CINDAS) of Purdue University. The development, contents, accessibility, and operation of the databases as well as the methodology for data evaluation, analysis, correlation, and synthesis used at CINDAS are presented and discussed.

INTRODUCTION

The Center for Information and Numerical Data Analysis and Synthesis (CINDAS) was founded at Purdue University on January 1, 1957, originally as the Thermophysical Properties Research Center (TPRC). Since its inception CINDAS has been conducting a systematic program for over 30 years on the properties of materials and has been developing comprehensive, high-quality, numerical databases on the properties of various classes of materials since 1972.

Some of the databases are developed as results of the operations by CINDAS of the information analysis centers of the U.S. Department of Defense (DoD), and the other databases are developed through the support of industrial organizations, research institutes, professional societies, and Purdue University.

The computerized numerical databases developed by CINDAS are interactive, menu-driven, and user-friendly. Since they are menu-driven, no special query language or commands need to be learned, and the databases are extremely easy to use. The databases are either for online operation and access through computer terminals and personal computers (PCs) with modems across the nation or for distribution on diskettes for use on personal computers.

As CINDAS has always considered the quality of the data in a database to be of utmost importance, major efforts have been devoted at CINDAS to the critical evaluation, analysis, correlation, and synthesis of the experimental data compiled from the worldwide literature to generate reliable reference data (recommended values).

SYSTEMATIC PROGRAM ON MATERIALS PROPERTIES

CINDAS has been conducting a comprehensive systematic program on the properties and behavior of materials since 1957. The program involves the basic and applied research; the cognizance and collection of relevant worldwide scientific and technical literature; the compilation, critical evaluation, analysis, correlation, and synthesis of experimental data to produce reliable reference data (recommended values); the generation of estimated values to fill data gaps and voids; the investigation of constitutive, structural, processing, environmental, ultrarapid heating, ultrarapid loading, and other effects on material properties and behavior; and the nationwide dissemination of the resulting data through publications and through user inquiry services.

Since 1972, CINDAS has been developing computerized numerical/technical databases on materials properties. The databases are either (1) for online operation and access through computer terminals and personal computers with modems across the nation or (2) for distribution of periodically updated PC-based databases on diskettes to qualified users for use on personal computers. Since 1988 CINDAS has been operating materials properties numerical databases to provide online numerical database service to U.S. Government agencies and laboratories, industrial organizations, and academic institutions. And since 1990 CINDAS has been distributing PC-based databases on diskettes.

OPERATION OF DOD INFORMATION ANALYSIS CENTERS ON MATERIALS PROPERTIES

CINDAS operates three DoD Information Analysis Centers for the U.S. Department of Defense:

(1) DoD High Temperature Materials–Mechanical, Electronic and Thermophysical Properties Information Analysis Center (HTMIAC)

(2) DoD Ceramics Information Analysis Center (CIAC)

(3) DoD Metals Information Analysis Center (MIAC)

High Temperature Materials Information Analysis Center (HTMIAC). HTMIAC serves as the DoD's central source of engineering data and technical information on high-temperature materials properties, especially the properties of aerospace structural composites, aerospace structural metals, and infrared detector/sensor materials. The material groups covered by HTMIAC are the following:

(1) carbon/carbon composites
(2) carbon/phenolic composites
(3) fiberglass/epoxy composites
(4) graphite/bismaleimide composites
(5) graphite/epoxy composites
(6) graphite/polyimide composites
(7) Kevlar/epoxy composites
(8) silica/phenolic composites
(9) selected aluminum alloys
(10) selected titanium alloys
(11) selected stainless steels
(12) selected infrared detector/sensor materials
(13) selected e-m transparent materials
(14) selected thin films

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The property groups covered by HTMIAC are as follows:
(1) thermophysical properties
(2) thermoradiative properties
(3) mechanical properties
(4) optical properties
(5) electronic properties
(6) ablation properties
(7) physical properties

A High-Temperature Materials Properties Database covering the above material groups and property groups has been developed by HTMIAC and has been operated online since 1988.

Ceramics Information Analysis Center (CIAC). CIAC serves as the DoD's central source of engineering and technical data and research and development information on monolithic ceramics and ceramic composites, hybrids, laminates, and coatings utilized in Defense systems and hardware. The material groups covered by CIAC are the following:
(1) monolithic ceramics
(2) ceramic composites
(3) ceramic hybrids
(4) ceramic laminates
(5) ceramic coatings
(6) reinforcing fibers
(7) composite joints
(8) nonstructural composites (piezoelectric ceramic materials and optical materials)

The property groups covered by CIAC are as follows:
(1) mechanical properties (as a function of composite architecture, temperature, and environmental conditions)
(2) thermophysical and other properties

The following information groups are also covered by CIAC:
(1) latest research and development concepts, results, and trends
(2) applications and processing of ceramics, and processing equipment
(3) measurement and testing of ceramics, and test methods
(4) quality control related to ceramics
(5) corrosion/deterioration detection, prevention, and control, and other environmental effects on ceramics and systems
(6) producers, suppliers, and specifications for ceramics

CIAC is in the process of preparing two numerical databases: Continuous Fiber Reinforced Ceramic Matrix Composites Properties Database and Whisker and Particulate Reinforced Ceramic Matrix Composites Properties Database.

Metals Information Analysis Center (MIAC). MIAC serves as the DoD's central source of engineering and technical data and research and development information on monolithic metals, metal alloys, intermetallic compounds, and coatings utilized in Defense systems and hardware. The material groups covered by MIAC are the following:
(1) monolithic metals
(2) metal alloys
(3) intermetallic compounds
(4) coatings
(5) metal joints
(6) welds

The property groups covered by MIAC are as follows:
(1) mechanical properties (as a function of temperature and environmental conditions)
(2) thermophysical and other properties

The following information groups are also covered by MIAC:
(1) latest research and development concepts, results, and trends
(2) applications and processing of metals, and processing equipment
(3) measurement and testing of metals, and test methods
(4) quality control related to metals
(5) corrosion/deterioration detection, prevention, and control, and other environmental effects on metals and systems
(6) producers, suppliers, and specifications for metals

MIAC is in the process of preparing two numerical databases: Intermetallic Alloys Properties Database and Aluminum–Lithium Alloys Properties Database.

Furthermore, CINDAS has been a component of the U.S. National Standard Reference Data System (NSRDS) of the National Institute of Standards and Technology (NIST) since 1964, responsible for generating reliable reference data on properties of various groups of materials.

DATA EVALUATION, ANALYSIS, CORRELATION, AND SYNTHESIS

Owing to the difficulties encountered in the accurate measurement of the properties of materials and in the adequate characterization of test specimens, especially solids, the property data recorded in the scientific and technical literature are often conflicting, widely diverging, and subject to large uncertainty. Indiscriminate use of literature data for design and engineering calculations without knowing their reliability is dangerous and may cause inefficiency or product failure, which at times can be disastrous. It is, therefore, very important to critically evaluate and analyze the available data and information, to give judgment on the reliability and accuracy of the data, and to generate recommended reference data.

The methodology basically involves critical evaluation of the validity of the available data and related information, judgment on the reliability and accuracy of the data, resolution and reconciliation of disagreements in conflicting data (distinguishing first the real difference in data due to sample difference from the disagreement in data due to experimental error), correlation of data in terms of various affecting parameters (sometimes in reduced forms using the principle of corresponding states), curve fitting with theoretical or empirical equations, synthesis of the often fragmentary data (sometimes by combining the available data with the values derived from the data on related properties or related materials) to generate a fuller range of coverage of internally consistent values, comparison of the resulting values with theoretical predictions or with results calculated from theoretical relationships, etc.

Considering the thermal conductivity data, for example, in the critical evaluation of the validity and reliability of a particular set of experimental data, the temperature dependence of the property data is examined, and any unusual dependence or anomaly is carefully investigated. The experimental technique is reviewed to see whether the actual boundary conditions in the measurement agreed with those assumed in the theoretical model used to define the property. It is ascertained whether all the stray heat flows and losses were prevented or minimized and accounted for. Furthermore, the reduction of the data is examined to see whether all the

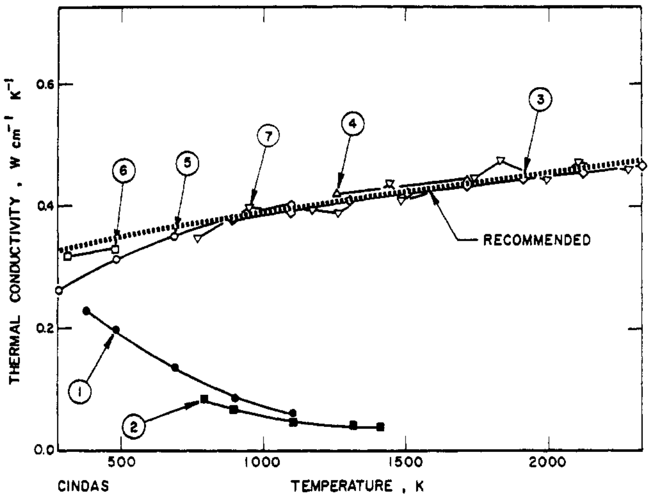

Figure 1. Experimental data and recommended values for the thermal conductivity of titanium carbide.

necessary corrections were appropriately applied, and the estimation of uncertainties is checked to ensure that all the possible sources of error, particularly systematic errors, were considered by the author(s).

Since the primary factor contributing to unreliable and erroneous experimental results is the systematic error in the measurements, experimental data can be judged to be reliable only if all sources of systematic error have been eliminated or minimized and accounted for. Considering the measurement of thermal transport properties such as thermal conductivity, for example, the major sources of systematic error may include at least the following:

(1) unsuitable experimental method
(2) poor experimental technique
(3) poor instrumentation and poor sensitivity of measuring circuits, sensors, or devices
(4) mismatch between actual experimental boundary conditions and those assumed in the theoretical model to derive the property value
(5) specimen and/or thermocouple chemical contamination
(6) unaccounted-for stray heat flows
(7) incorrect form factor for the measuring apparatus

As an example to illustrate CINDAS' work on the critical evaluation and analysis of experimental data, Figure 1 shows the available experimental data on titanium carbide, in which the lower data are about five times lower than the upper data at 800 K and are about 10 times lower at 1350 K. CINDAS' recommended values are also shown in the figure. The lower two sets of data were published in 1954 and were obtained by using two completely different experimental methods and seem to confirm each other. These lower data were the only data available before 1961, and machine tool designers might have used these erroneous data for years since titanium carbide has been extensively used to make machine tools. One can imagine the consequence of using 10-times-lower values for designing a machine tool or anything. Since 1961, newer measurements indicate that the thermal conductivity of titanium carbide is actually increasing with temperature, instead of decreasing when the temperature increases as indicated by the lower two sets of data, and the true values are so much higher. It is easy to prove that the lower data are wrong by a simple analysis.

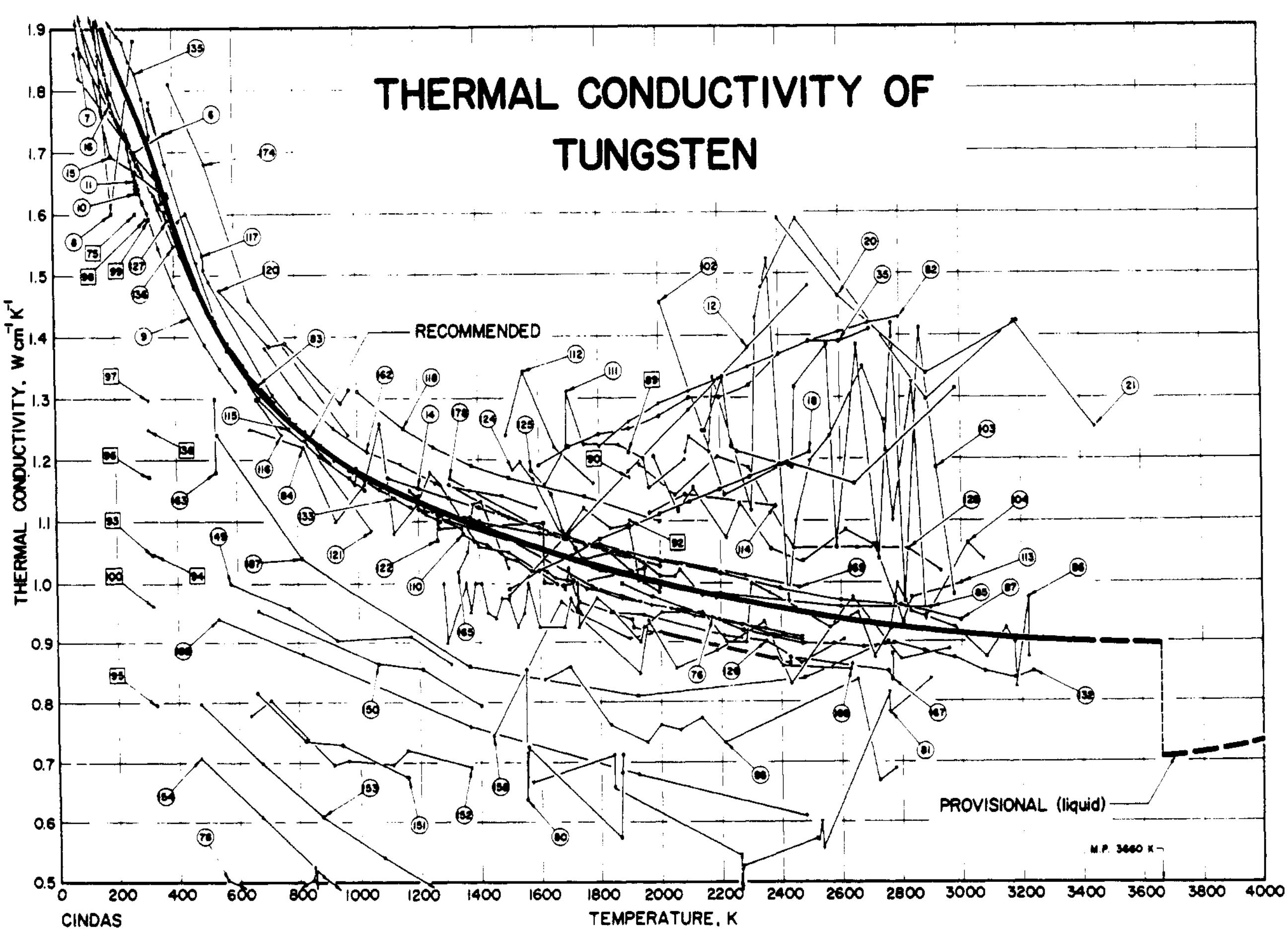

Figure 2. Experimental data and recommended values for the thermal conductivity of tungsten.

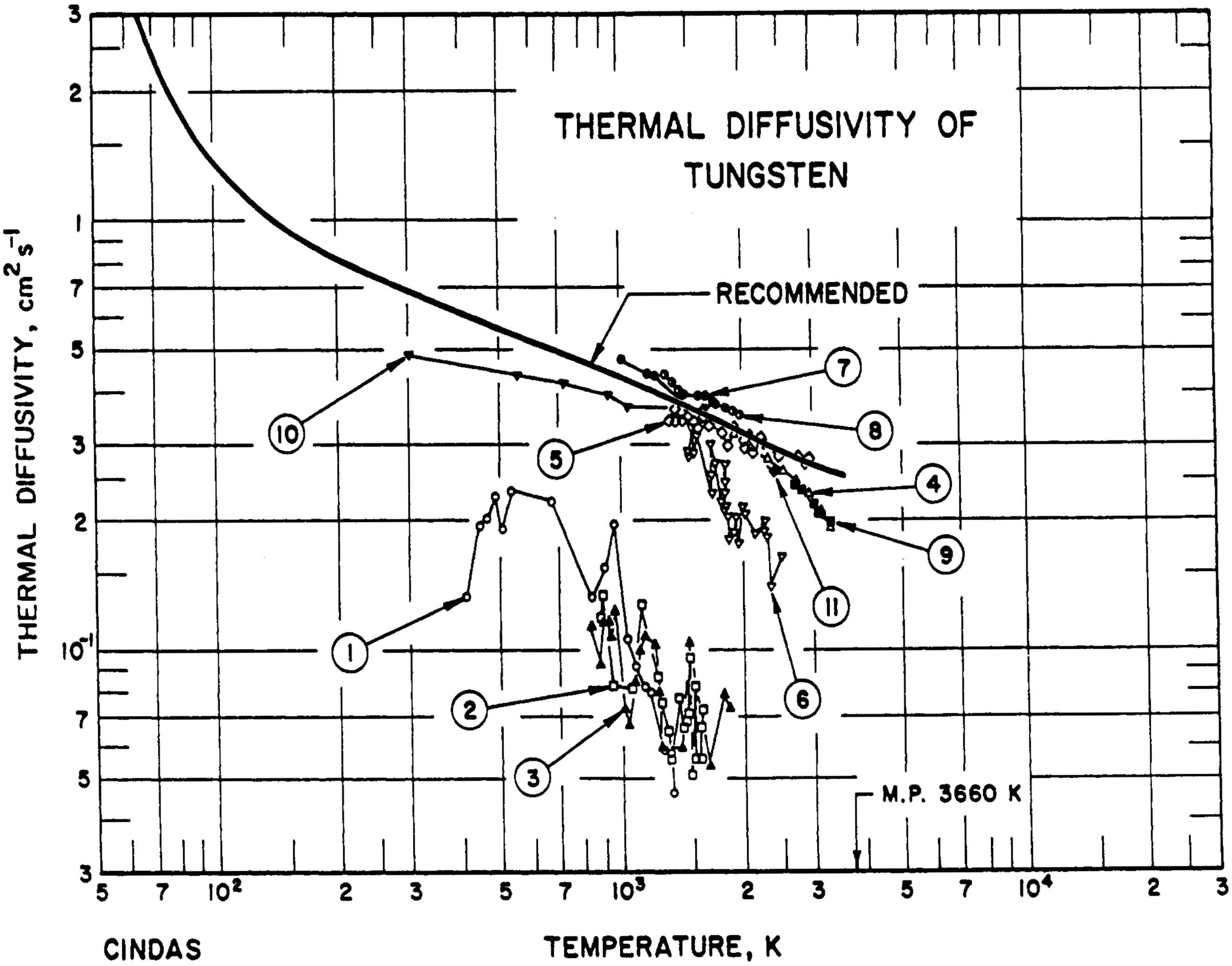

Figure 3. Experimental data and recommended values for the thermal diffusivity of tungsten.

The total thermal conductivity, λ, of an electrically conducting material such as titanium carbide consists of two components: an electronic component, λ_e, and a lattice component, λ_g. λ_e may be calculated from electrical resistivity data, and the resulting calculated values for λ_e of titanium carbide are much higher than the lower two sets of data in Figure 1, which are for the total thermal conductivity, λ. Since the whole must be greater than a part, λ must be greater than λ_e. This proves that the lower data, which are for λ but much smaller than λ_e, are impossible.

Another example for illustration of data evaluation and analysis is the thermal conductivity of tungsten, for which a part of the available experimental data and CINDAS' recommended values are shown in Figure 2.[1] It can be observed from Figure 2 that a large portion of the experimental data are conflicting, widely diverging, and subject to large uncertainty, and that the spread of data is over 300%. It has been estimated that the cost of experimental research is over $50 000 per published research paper. Since the number of published papers reporting experimental results on the thermal conductivity of tungsten is more than 300, a total of over $15 000 000 in research funds had been spent to produce the confusion of experimental data shown in Figure 2. The true values of the thermal conductivity of tungsten had not been known even with the $15 000 000 spent on research and the availability of over 300 publications reporting experimental data beginning in 1914 until CINDAS critically evaluated and analyzed the discordant experimental data and generated the recommended reference values as shown in the figure at an extremely small fraction of the cost. These CINDAS' recommended values have been recognized as national standard reference data.

Similarly, Figure 3 shows the available experimental data and CINDAS' recommended values for the thermal diffusivity of tungsten.[2] The lower portion of the experimental data are utterly erroneous, being about five times too low. The recommended curve shown in the figure not only gives the correct thermal diffusivity values for tungsten but also covers a full range of temperature, going far beyond the limited range covered by the discordant experimental data.

CINDAS' work on the correlation and synthesis of experimental data is illustrated by Figures 4–8. Figure 4 shows the available experimental data on the thermal conductivity of aluminum + copper alloys, which are very limited and fragmentary. Based on the results of evaluation and analysis of these thermal conductivity data and on CINDAS' recommended values for the electrical resistivity and the thermoelectric power of these alloys, the full-range recommended values for the thermal conductivity of these alloys were generated as shown in Figure 5.[3] The merit of data synthesis can best be appreciated by comparing the available few experimental data shown in Figure 4 and the full-range recommended values presented in Figure 5.

The available experimental data on the thermoelectric power of nickel + copper alloys are shown in Figure 6. From these limited fragmentary data, recommended values were generated

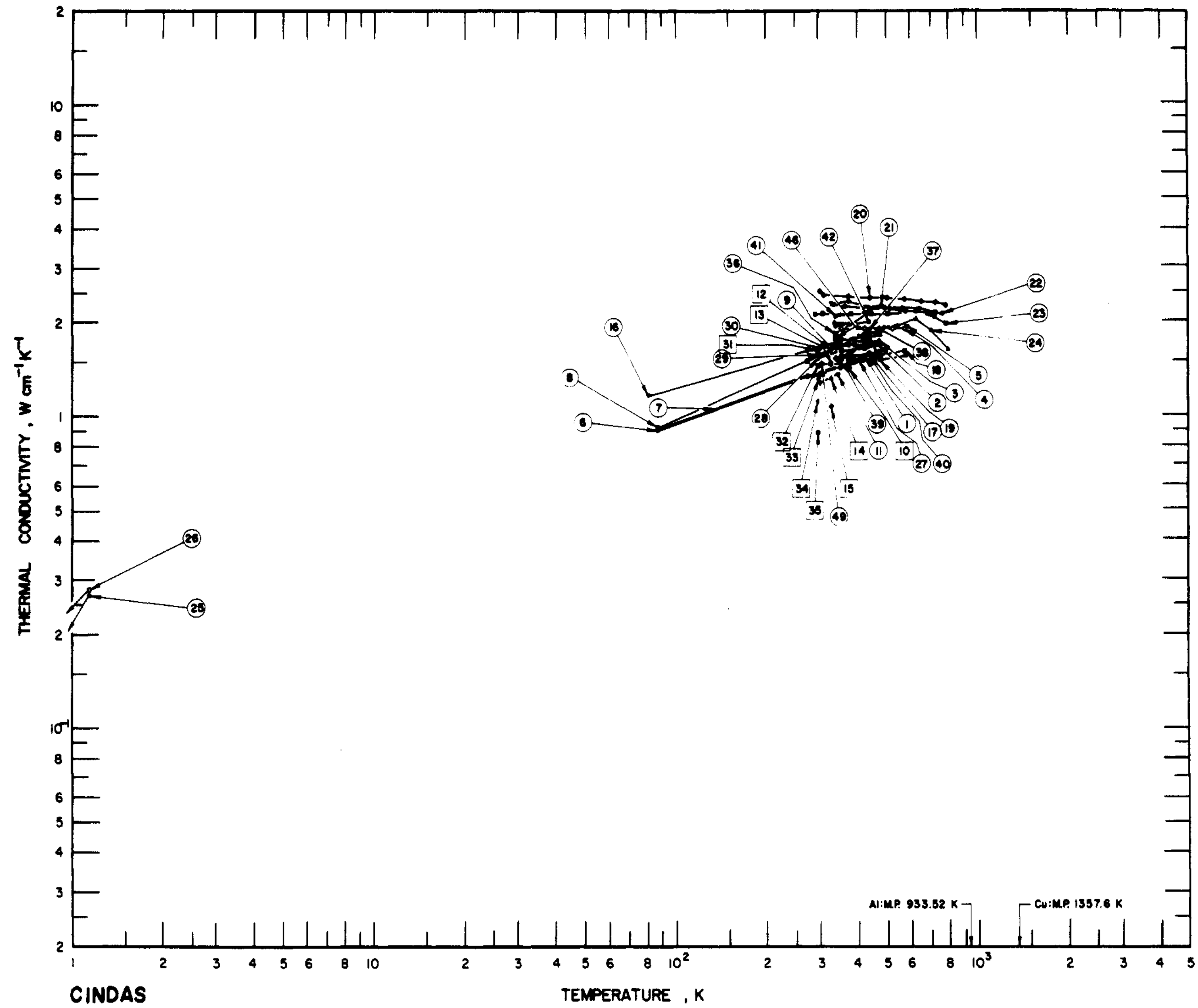

Figure 4. Experimental data on the thermal conductivity of aluminum + copper alloys.

to cover a full range of temperatures and composition as shown in Figure 7.[4] Figure 8 shows the recommended values for the thermoelectric power of the copper-nickel alloy system (including both copper + nickel alloys and nickel + copper alloys) as a function of composition at various temperatures.[4]

FEATURES OF COMPUTERIZED NUMERICAL DATABASES AT CINDAS

The computerized numerical databases on materials property data at CINDAS/Purdue University include both online databases and PC-based databases. Both kinds of databases are interactive, menu-driven, and user-friendly. No special query language or commands need to be learned by the users, and the databases are extremely easy to use. Numerical data are retrievable in graphical as well as tabular forms. The databases permit both the direct mode of search/retrieval of data for specified materials, properties and independent variables and the inverted mode of search/retrieval of qualified materials that meet a set of specified properties requirements (which is the computer-aided materials selection). They also permit online interactive manipulation of the retrieved data such as units conversion, variable transformation, etc.

Both kinds of databases are managed and operated by using CINDAS' own proprietary database management system (DBMS) software, and no commercial third-party software is required.

COMPUTERIZED NUMERICAL DATABASES AT CINDAS/PURDUE UNIVERSITY

The following computerized numerical databases have been developed:

(1) High Temperature Materials Properties Database (online operated since 1988)

(2) Dielectric Materials Database (online operated since 1988)

(3) Microelectronics Packaging Materials Database (distributed on diskettes for use on personal computers since 1990)

(4) Database for Laser Effects (distributed on diskettes for use on personal computers since 1990)

(5) Thermophysical properties of Solids Database (partially online operational)

(6) Military Standardization Handbook 5 (Metallic Materials and Elements for Aerospace Vehicle Structures) Database

(7) Thermophysical Properties of Fluids Database

(8) Rocks and Minerals Properties Database

As discussed in the section on the operation of the DoD information analysis centers on materials properties, the

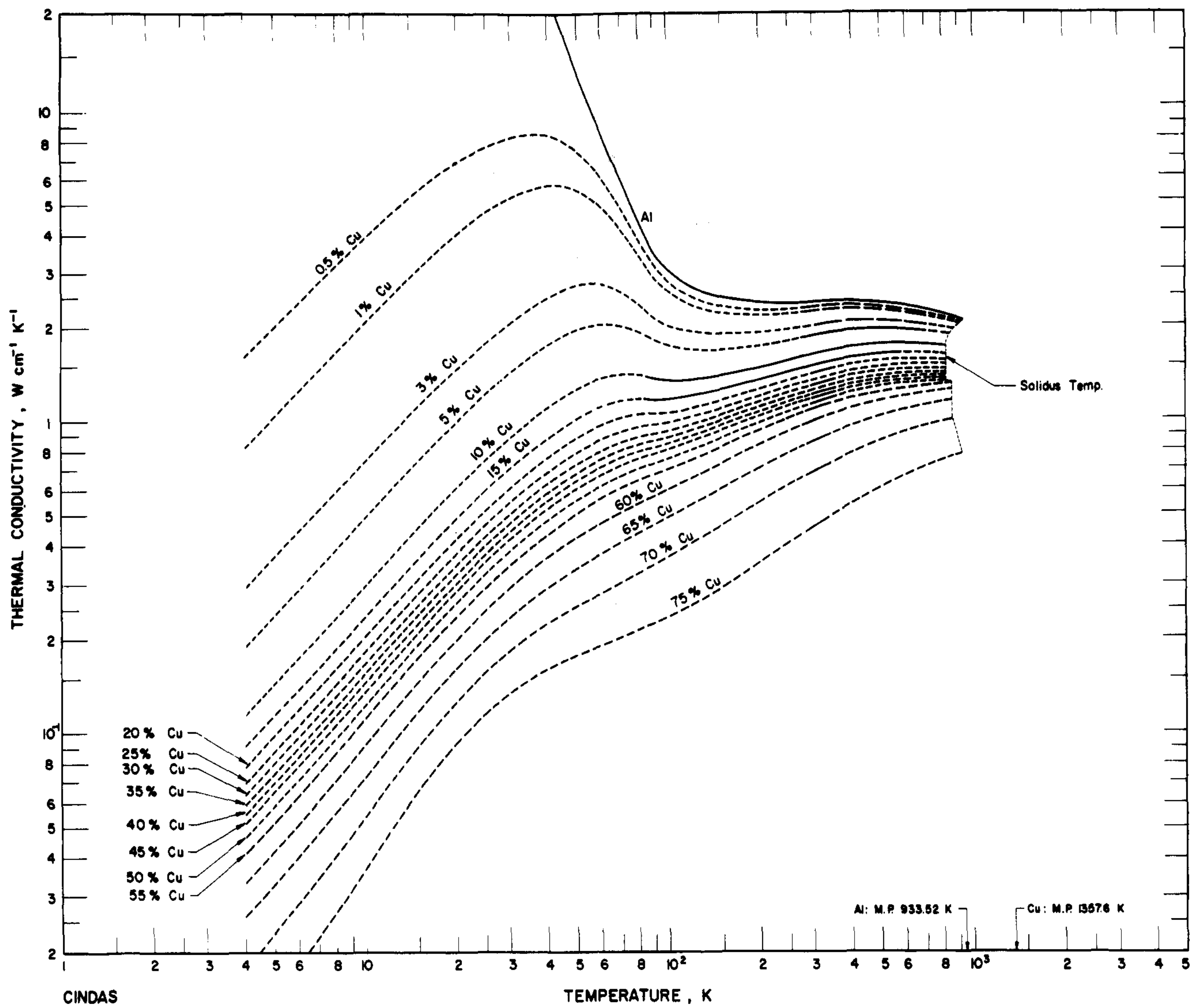

Figure 5. Recommended values for the thermal conductivity of aluminum + copper alloys.

following numerical databases are under development:

(1) Continuous Fiber Reinforced Ceramic Matrix Composites Properties Database

(2) Whisker and Particulate Reinforced Ceramic Matrix Composites Properties Database

(3) Intermetallic Alloys Properties Database

(4) Aluminum–Lithium Alloys Properties Database

The contents of the operational databases are discussed below.

High-Temperature Materials Properties Database. This database is produced as a result of the operation of HTMIAC by CINDAS for the DoD and contained 22 028 sets of data as of March 31, 1992, including 17 491 sets of unrestricted data in an online database and 4537 sets of restricted data in a controlled database. These data cover 720 materials, 231 properties, 342 parameters, and 108 independent variables. The online database has been operated since 1988 from a host computer at CINDAS/Purdue University to provide online numerical database service to HTMIAC users. Please contact CINDAS for requesting online access to this database.

The materials covered are 405 varieties of aerospace structural composites (including 23 varieties of carbon/carbon composites, 61 varieties of carbon/phenolic composites, 65 varieties of fiberglass/epoxy composites, 12 varieties of graphite/bismaleimide composites, 142 varieties of graphite/epoxy composites, 25 varieties of graphite/polyimide composites, 54 varieties of Kevlar/epoxy composites, 17 varieties of silica/phenolic composites, and 6 varieties of nylon/phenolic composites), 126 varieties of composite constituents, 107 varieties of aerospace structural alloys, 64 varieties of infrared detector/sensor materials, and 18 other materials (including 3 varieties of alumina, 3 varieties of boron nitride, 9 varieties of graphite, 1 polycarbonate, and 2 elemental metals).

The properties covered are 48 thermophysical and thermoradiative properties, 22 electronic, electrical, and optical properties, and 161 mechanical properties. The parameters covered include 199 general parameters, 118 construction configuration parameters for composite materials, and 25 material environment parameters.

Since material property data are meaningful only if adequate information on the test material and on the property measurement is also provided, each set of data in this database consists of numerical data points (as a function of temperature and/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, specimen geometry and dimensions, material history, heat treatment, surface condition, producer,

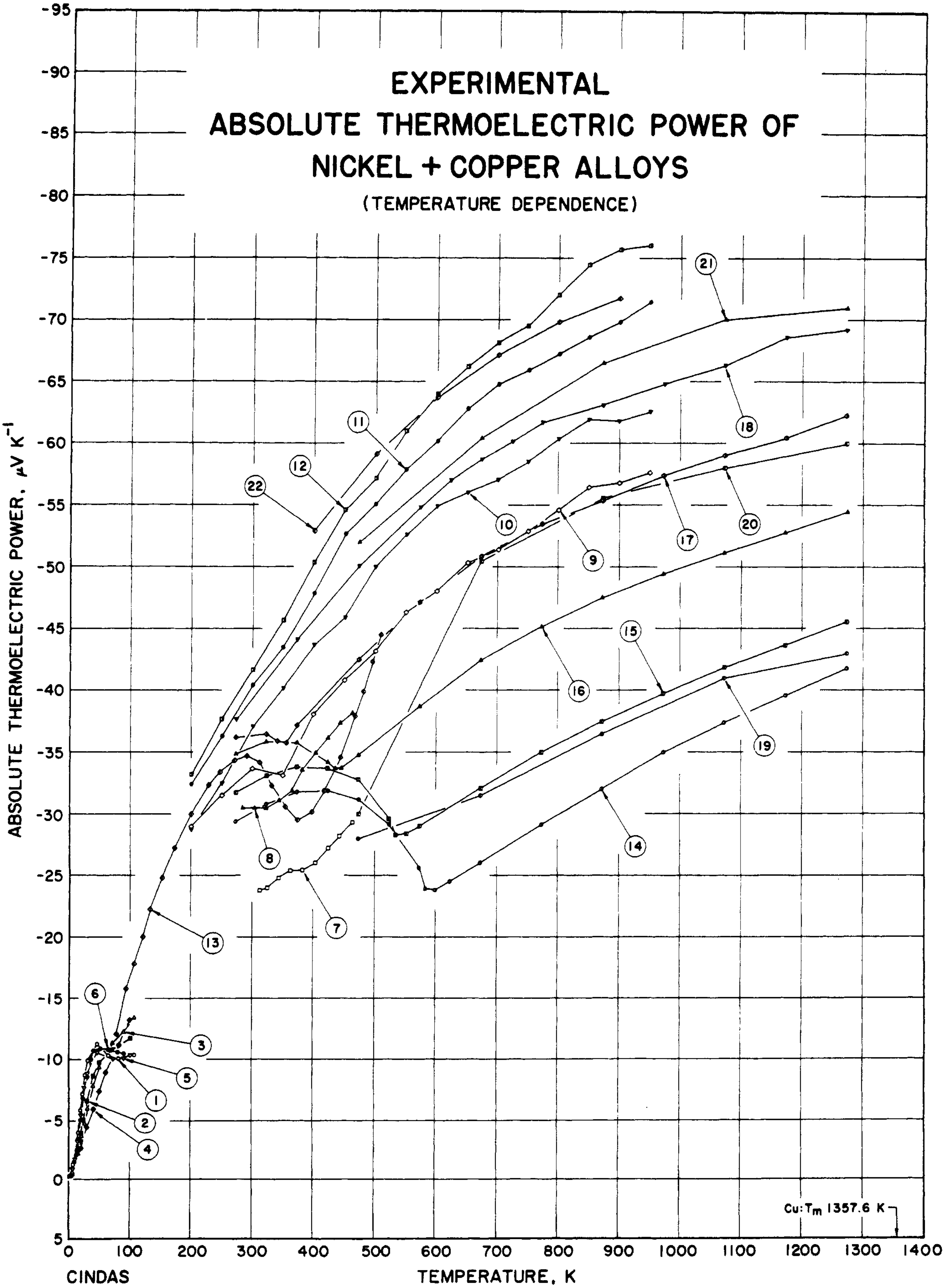

Figure 6. Experimental data on the absolute thermoelectric power of nickel + copper alloys.

supplier, method of measurement, test environment, heat flow direction, heating rate, heat-up time, heat-up temperature, holding time at temperature, type of heat source, and loading rate, insofar as these are contained in the original document.

A sample of data contained in this database is shown in the Appendix.

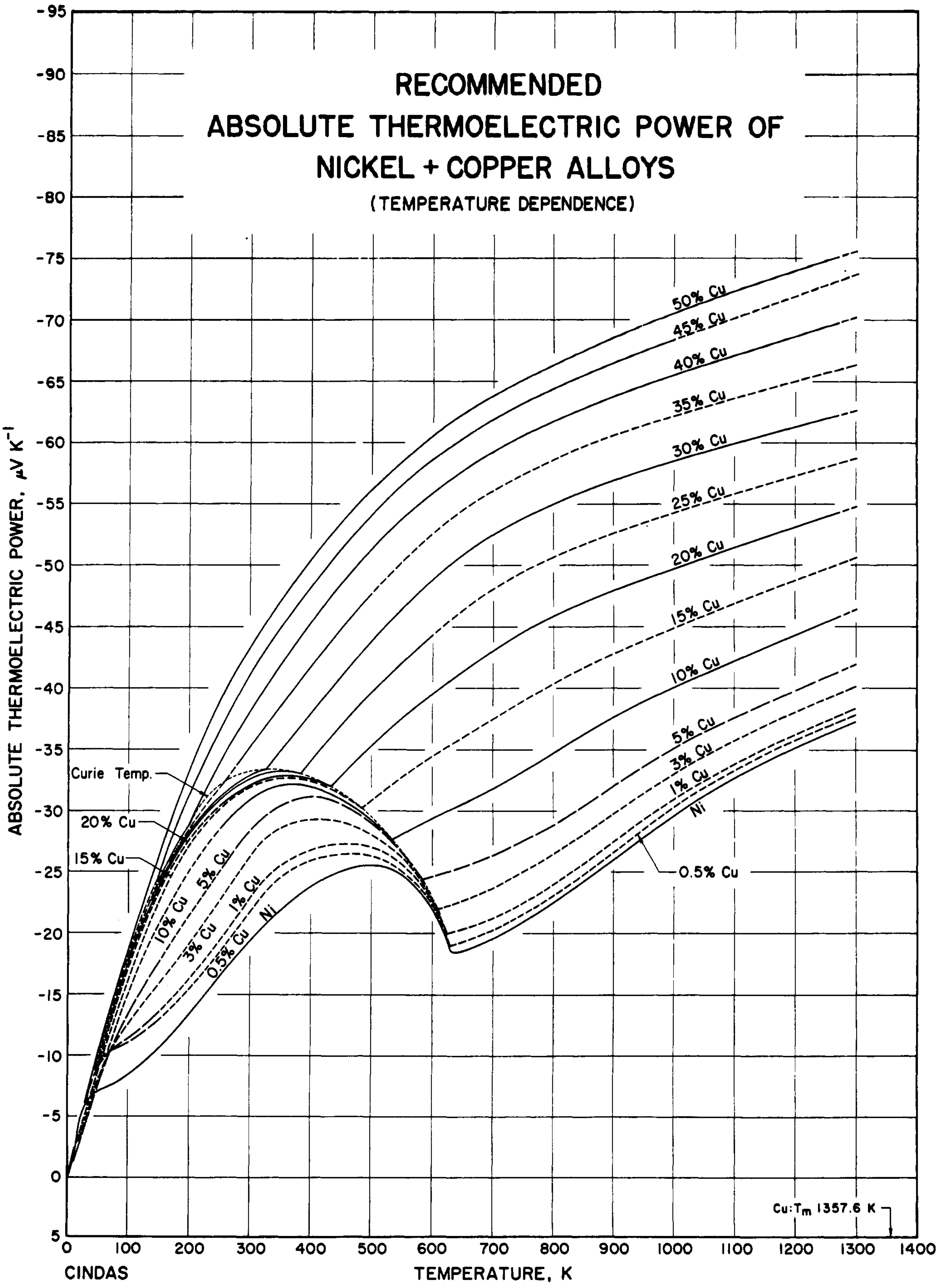

Figure 7. Recommended values for the absolute thermoelectric power of nickel + copper alloys.

Dielectric Materials Database. This online database was developed under the sponsorship of the Electric Power Research Institute (EPRI) and has been online operated since 1990. As of December 31, 1991, it contained 15 700 sets of data and 17 500 entries of dielectric materials producers' specification data, which cover 1200 electrical insulating solids,

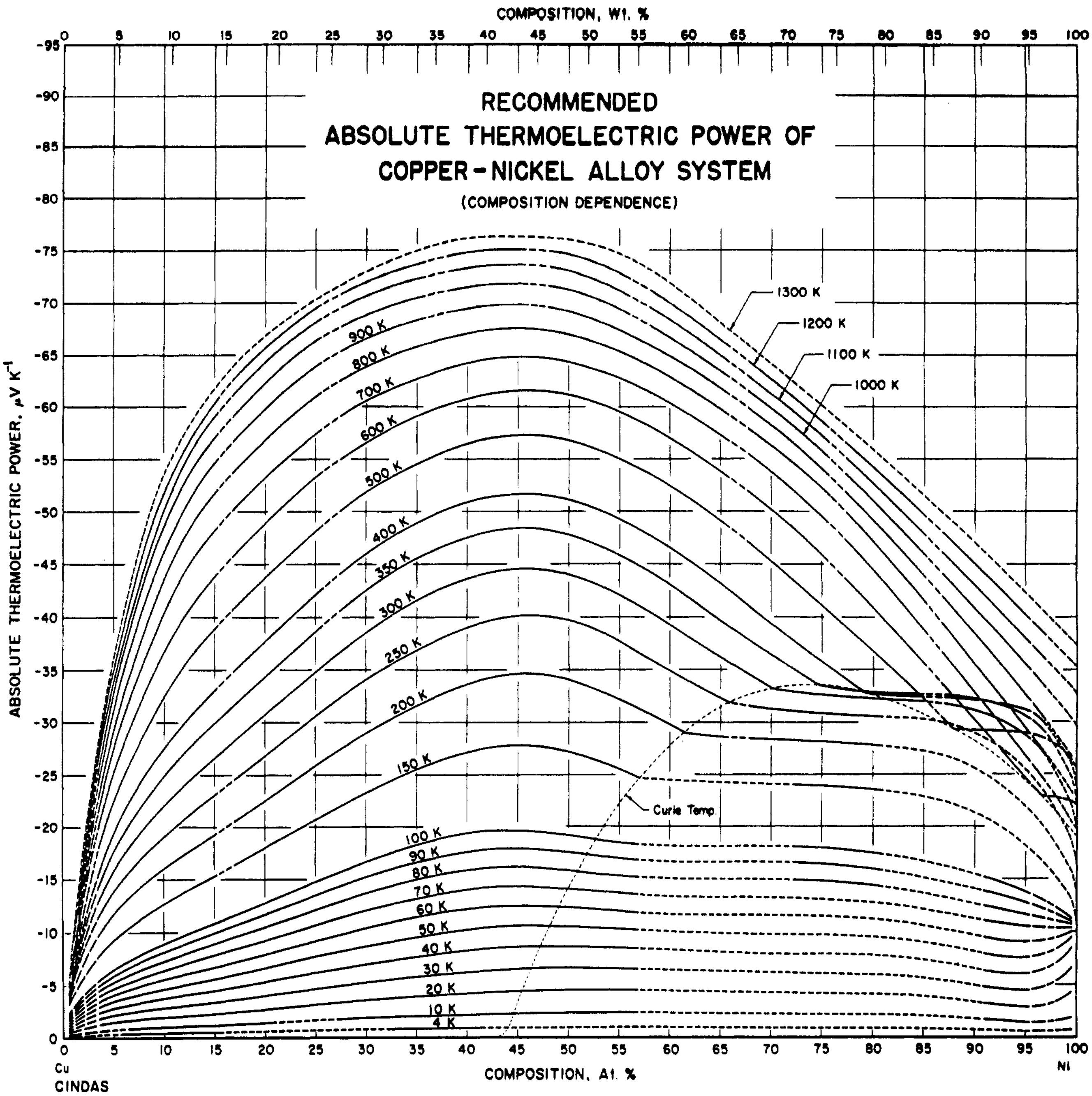

Figure 8. Recommended values for the absolute thermoelectric power of copper-nickel alloy systems.

liquids, gases, and combinations thereof, 284 properties, and 122 independent variables. Please contact CINDAS for requesting online access to this database.

Dielectric material groups covered by this database are the following:

(1) acetal resins
(2) acrylic resins
(3) alkyl resins
(4) cellulose polymers
(5) ceramics
(6) porcelains
(7) glasses
(8) elastomers/rubbers
(9) epoxy resins
(10) fluorocarbon polymers
(11) formaldehydes
(12) laminates
(13) mica
(14) papers
(15) paper laminates
(16) phenolics
(17) polyamides
(18) polycarbonates
(19) polyesters
(20) polyethylenes
(21) polyimides
(22) polyimide composites
(23) polypropylenes
(24) polyphenylene compounds
(25) polystyrenes
(26) polysulfone polymers
(27) polyurethanes
(28) polyvinyl compounds
(29) polyxylylenes
(30) silicone resins
(31) hydrocarbons
(32) synthetic hydrocarbons
(33) chlorinated hydrocarbons

(34) fluorocarbons
(35) silicone oils
(36) retrofilling fluids
(37) organic esters
(38) ethers
(39) liquid gases
(40) vegetable oils
(41) air
(42) elemental gases
(43) sulfur hexafluoride
(44) freons
(45) gaseous mixtures

Property and information groups covered are as follows:

(1) electrical properties
(2) physical properties
(3) chemical properties
(4) thermal properties
(5) optical properties
(6) mechanical properties
(7) flammability properties
(8) aging and degradation
(9) health hazards and environmental effects
(10) processability
(11) producers, suppliers, and availability
(12) recommended applications

Microelectronic Packaging Materials Database. This is a PC-based numerical database developed under the sponsorship of the Semiconductor Research Corporation (SRC). It is updated three times a year and has been distributed on diskettes since 1990 for use on personal computers.

This database contains data on the mechanical, thermal, electrical, and physical properties of thin-film, thin-wire, and bulk packaging materials, including metals, alloys, semiconductors, ceramics, polymers, composites, fluids, etc. and serves the needs of the semiconductor/electronics industry by providing reliable data on packaging materials for microelectronics packaging applications.

Database for Laser Effects. This PC-based Database for Laser Effects contains data on high-energy laser materials interaction effects and also data on the properties of the laser-tested materials. Operating in a classified mode, this database has been distributed since 1990 on diskettes to interested and authorized users with security clearance and classified facility for use on personal computers.

Thermophysical Properties of Solids Database. This database is the computerized version of the 10 volumes on solids of CINDAS' 13-volume *Thermophysical Properties of Matter—The TPRC Data Series*[5] and several subsequent CINDAS databook publications. It contains about 44 000 sets of data covering the thermophysical and thermoradiative properties of about 6400 solid materials.

Materials groups covered are the following:

(1) metallic elements
(2) graphites and nonmetallic elements
(3) ferrous alloys (15 groups)
(4) nonferrous alloys (41 groups)
(5) intermetallic compounds
(6) inorganic compounds
(7) organic compounds
(8) ceramics
(9) cermets
(10) glasses
(11) polymers
(12) composites
(13) applied coatings
(14) mixtures
(15) insulations
(16) concretes, bricks, and other building materials
(17) natural substances and their derivatives
(18) biological materials

Thermophysical and thermoradiative properties covered are as follows:

(1) thermal conductivity
(2) thermal diffusivity
(3) thermal expansion
(4) specific heat
(5) thermal emittance
(6) thermal reflectance
(7) thermal absorptance
(8) thermal transmittance

Supplementary Material Available: Sample data in the high-temperature materials property database (5 pages). Ordering information is given on any current masthead page.

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