N94-25123

Establishment of Computerized Numerical Databases on Thermophysical and Other Properties of Molten as well as Solid Materials and Data Evaluation and Validation for Generating Recommended Reliable Reference Data

by

C.Y. Ho*
Center for Information and Numerical Data Analysis and Synthesis (CINDAS)
Purdue University
West Lafayette, IN 47906-1398

Abstract

The Center for Information and Numerical Data Analysis and Synthesis, (CINDAS), measures and maintains databases on thermophysical, thermoradiative, mechanical, optical, electronic, ablation, and physical properties of materials.Emphasis is on aerospace structural materials especially composites and on infrared detector/sensor materials. Within CINDAS, the Department of Defense sponsors at Purdue several centers: the High Temperature Material Information Analysis Center (HTMIAC), the Ceramics Information Analysis Center (CIAC) and the Metals Information Analysis Center (MIAC). The responsibilities of CINDAS are extremely broad encompassing basic and applied research, measurement of the properties of thin wires and thin foils as well as bulk materials, acquisition and search of world-wide literature, critical evaluation of data, generation of estimated values to fill data voids, investigation of constitutive, structural, processing, environmental, and rapid heating and loading effects, and dissemination of data. Liquids, gases, molten materials and solids are all considered.

The responsibility of maintaining widely used databases includes data evaluation, analysis, correlation, and synthesis. material property data recorded on the literature are often conflicting, diverging and subject to large uncertainties. it is admittedly difficult to accurately measure materials properties. Systematic and random errors both enter. Some errors result from lack of characterization of the material itself (impurity effects). In some cases assumed boundary conditions corresponding to a theoretical model are not obtained in the experiments. Stray heat flows and losses must be accounted for. some experimental methods are inappropriate and in other cases appropriate methods are carried out with poor technique. Conflicts in data may be resolved by curve fitting of the data to theoretical or empirical models or correlation in terms of various affecting parameters. Reasons (e.g. phase transitions) must be found for unusual dependence or any anomaly. Such critical evaluation involves knowledge of theory, experience in measurement, familiarity with metallurgy (microstructural behavior) and not inconsiderable judgement.

An examination of typical data compiled and analyzed by CINDAS shows that the ther-

mal conductivity of a material reported in the literature may vary by a factor of two or more; the range of reported values increases as temperature increases reflecting the difficulty of high temperature measurements. Often only estimates of melt behavior are available, despite the importance of melt properties in modelling, welding or other solidification processes. There may be only a few measurements available for properties such as kinematic viscosity, even for widely used materials such as stainless steel. In the face of such a paucity of existing data and in a national environment where too few new data are being generated it is nonetheless the responsibility of CINDAS to select and disseminate recommended values of a wide variety of thermophysical properties.

* Extended abstract written by Mr. Thomas Glasgow.

CENTER FOR INFORMATION AND NUMERICAL DATA ANALYSIS AND SYNTHESIS (CINDAS)

* Founded at Purdue University on 1 January 1957 as a Materials Properties Research Center -- originally called the Thermophysical Properties Research Center (TPRC)

* Conducting a Comprehensive Systematic Program on the Thermophysical, Thermoradiative, Mechanical, Electronic, Optical, and Other Properties of Materials

* Operating for the U.S. Department of Defense (DoD):
  - DoD High Temperature Materials - Mechanical, Electronic and Thermophysical Properties Information Analysis Center (HTMIAC)
  - DoD Ceramics Information Analysis Center (CIAC)
  - DoD Metals Information Analysis Center (MIAC)

CENTER FOR INFORMATION AND NUMERICAL DATA ANALYSIS AND SYNTHESIS (CINDAS) (Continued)

* Developing Computerized Bibliographic Databases since 1966 and Computerized Numerical Databases since 1972

* Possessing the Largest Numerical Database System on the Properties of Solid Materials

* Publishing Over 70 Volumes of Books on Materials Properties Data and Information

* Having 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 the Properties of Various Groups of Materials such as Elements, Alloys, Compounds, and Fluids

OPERATION OF THE DOD HIGH TEMPERATURE MATERIALS - MECHANICAL, ELECTRONIC AND THERMOPHYSICAL PROPERTIES 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 and metals and infrared detector/sensor materials

* Property Groups Covered
  - Thermophysical properties
  - Thermoradiative properties
  - Mechanical properties
  - Optical properties
  - Electronic properties
  - Ablation properties
  - Physical properties

OPERATION OF THE DOD HIGH TEMPERATURE MATERIALS - MECHANICAL, ELECTRONIC AND THERMOPHYSICAL PROPERTIES INFORMATION ANALYSIS CENTER (HTMIAC) (Continued)

* Material Groups Covered
  - Carbon/carbon composites
  - Carbon/phenolic composites
  - Fiberglass/epoxy composites
  - Graphite/bismaleimide composites
  - Graphite/epoxy composites
  - Graphite/polyimide composites
  - Kevlar/epoxy composites
  - Silica/phenolic composites
  - Selected aluminum alloys
  - Selected titanium alloys
  - Selected stainless steels
  - Selected infrared detector/sensor materials
  - Selected e-m transparent materials
  - Selected thin films

OPERATION OF THE DOD 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

* Material Groups Covered
  - Monolithic metals
  - Metal alloys
  - Intermetallic compounds
  - Coatings
  - Metal joints
  - Welds

OPERATION OF THE DOD METALS INFORMATION ANALYSIS CENTER (MIAC) (Continued)

* Property Groups Covered
  - Mechanical properties (as a function of temperature and environmental conditions)
  - Thermophysical and other properties

* Information Covered
  - Latest research and development concepts, results, and trends
  - Applications and processing of metals, and processing equipment
  - Measurement and testing of metals, and test methods
  - Quality control related to metals
  - Corrosion/deterioration detection, prevention and control, and other environmental effects on metals and systems
  - Producers, suppliers, and specifications for metals

OPERATION OF THE DOD 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

* Material Groups Covered
  - Monolithic ceramics
  - Ceramic composites
  - Ceramic hybrids
  - Ceramic laminates
  - Ceramic coatings
  - Reinforcing fibers and whiskers
  - Composite joints
  - Non-structural composites (piezoelectric-ceramic materials and optical materials)

OPERATION OF THE DOD CERAMICS INFORMATION ANALYSIS CENTER (CIAC) (Continued)

* Property Groups Covered
  - Mechanical properties (as a function of composite architecture, temperature, and environmental conditions)
  - Thermophysical and other properties

* Information Covered
  - Latest research and development concepts, results, and trends
  - Applications and processing of ceramics, and processing equipment
  - Measurement and testing of ceramics, and test methods
  - Quality control related to ceramics
  - Corrosion/deterioration detection, prevention and control, and other environmental effects on ceramics and systems
  - Producers, suppliers, and specifications for ceramics

CINDAS' COMPREHENSIVE SYSTEMATIC PROGRAM ON THE PROPERTIES OF MATERIALS

* Basic and Applied Research
* Measurement of the Properties of Thin Wires and Thin Foils as well as Bulk Materials
* Search and Acquisition of Relevant Worldwide Scientific and Technical Literature
* Data Extraction, Compilation, Critical Evaluation, Analysis, Correlation, and Synthesis
* Generation of Recommended Values as Reliable Reference Data
* Generation of Estimated Values to Fill Data Gaps and Voids
* Investigation of Constitutive, Structural, Processing, Environmental, Rapid Heating, and Rapid Loading Effects on Material Properties

CINDAS' COMPREHENSIVE SYSTEMATIC PROGRAM ON THE PROPERTIES OF MATERIALS (Continued)

* Dissemination of Resulting Data through Publications and User Inquiry Services
* Computerization of Resulting Data to Establish Computerized Numerical Databases
* Operation of an Online Numerical Database System on Materials Properties to Provide Online Numerical Database Service to U.S. Government Agencies and Laboratories and to Industrial Organizations
* Distribution of PC-based Databases on Diskettes for Use on Personal Computers

DATA COMPILATION, EVALUATION, VALIDATION, ANALYSIS, AND SYNTHESIS

* Aiming at Generating Recommended Reliable Reference Data
* Covering Liquids, Gases, Molten Materials, as well as Solid Materials
* Covering Thermophysical, Thermoradiative, Optical, Electronic, Mechanical, and Other Properties If and When Appropriate

DATA EVALUATION, ANALYSIS, CORRELATION, AND SYNTHESIS

* Why?
  - Material property data recorded in the literature are often conflicting, diverging, and subject to large uncertainty, owing to the difficulties encountered in
    - the accurate measurement of material properties
    - the adequate characterization of test materials, especially solids
  - Quality of the data in a database is of utmost importance

DATA EVALUATION, ANALYSIS, CORRELATION, AND SYNTHESIS (Continued)

* How?
  - Critical evaluation of the validity of the available data and related information
  - Judgment on the reliability and accuracy of the data
  - Detection of systematic errors from random errors in property measurement
  - Distinguishing of the real difference in data due to sample difference from the disagreement in data due to experimental error
  - Resolution and reconciliation of disagreements in conflicting data

DATA EVALUATION, ANALYSIS, CORRELATION, AND SYNTHESIS (Continued)

* How? (continued)
  - 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 fragmentary data into internally consistent values (sometimes by combining the available data with values derived from the data on related properties or related materials)
  - Comparison of the resulting values with theoretical predictions or with results calculated from theoretical relationships

CRITICAL EVALUATION OF THERMAL CONDUCTIVITY DATA, FOR EXAMPLE

* Examine the Temperature Dependence of the Property Data and Carefully Investigate Any Unusual Dependence or Anomaly

* Review the Experimental Technique to See Whether the Actual Boundary Conditions in the Measurement Agreed with Those Assumed in the Theoretical Model Used to Define the Property

* Ascertain Whether All the Stray Heat Flows and Losses Were Prevented or Minimized and Accounted for

* Examine the Reduction of Data to See Whether All the Necessary Corrections Were Appropriately Applied

* Check the Estimation of Uncertainties to Ensure that All the Possible Sources of Errors, Particularly Systematic Errors, Were Considered by the Author(s)

BEWARE OF SYSTEMATIC ERRORS

* The Primary Factor Contributing to Unreliable and Erroneous Experimental Results Is the Systematic Errors in the Measurement

* Experimental Data May Possibly Be Judged to Be Reliable Only if All Sources of Systematic Errors Have Been Eliminated or Minimized and Accounted for

MAJOR SOURCES OF SYSTEMATIC ERRORS IN THE MEASUREMENT OF THERMAL TRANSPORT PROPERTIES

* Unsuitable Experimental Method

* Poor Experimental Technique

* Poor Instrumentation and Poor Sensitivity of Measuring Circuits, Sensors, or Devices

* Mismatch between Actual Experimental Boundary Conditions and Those Assumed in the Theoretical Model to Derive the Property Value

* Specimen and/or Thermocouple Chemical Contamination

* Unaccounted-For Stray Heat Flows

* Incorrect Form Factor for the Measuring Apparatus

THERMOPHYSICAL PROPERTIES OF SOLIDS DATABASE

* This is a Computerized, Online, Numerical Database
* Contains About 44,000 Sets of Data Covering the Thermophysical and Thermoradiative Properties of About 6,400 Solid Materials
* Properties Covered:
  - Thermal conductivity
  - Thermal diffusivity
  - Thermal expansion
  - Specific heat
  - Thermal emittance
  - Thermal reflectance
  - Thermal absorptance
  - Thermal transmittance

THERMOPHYSICAL PROPERTIES OF SOLIDS DATABASE (Continued)

* Material Groups Covered:
  - Metallic elements
  - Graphites and nonmetallic elements
  - Ferrous alloys (15 groups)
  - Nonferrous alloys (41 groups)
  - Intermetallic compounds
  - Inorganic compounds
  - Organic compounds
  - Ceramics
  - Cermets
  - Glasses
  - Polymers
  - Composites
  - Applied coatings
  - Mixtures
  - Insulations
  - Concretes, bricks, and other building materials
  - Natural substances and their derivatives
  - Biological materials

HIGH TEMPERATURE MATERIALS PROPERTIES DATABASE (Continued)

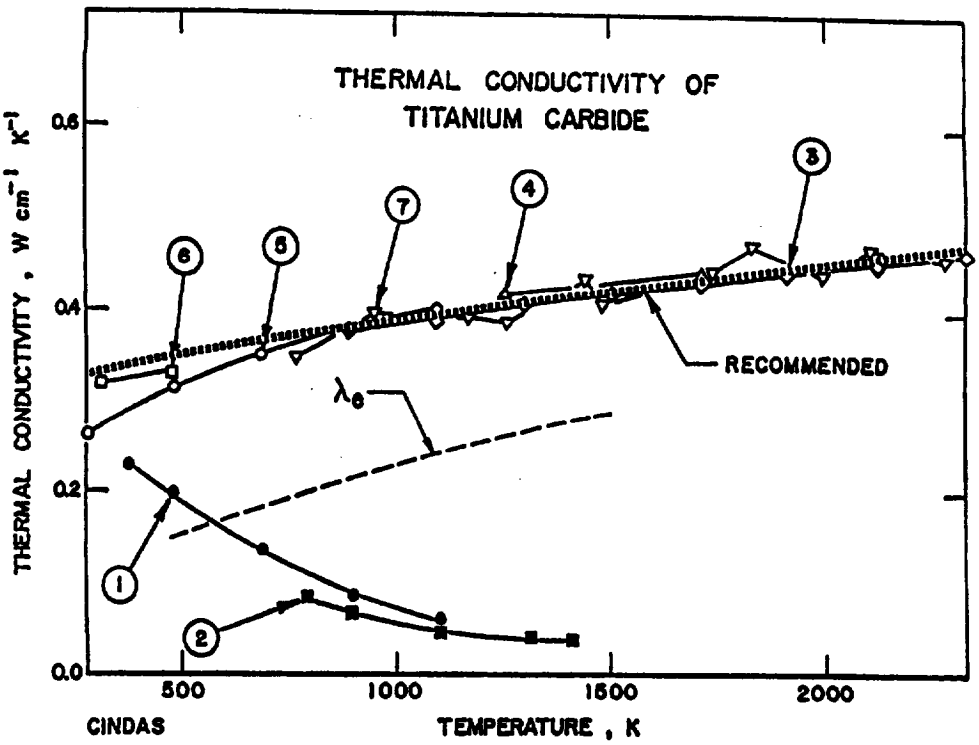
* Material Groups Covered:
  - Carbon/carbon composites
  - Carbon/phenolic composites
  - Fiberglass/epoxy composites
  - Graphite/bismaleimide composites
  - Graphite/epoxy composites
  - Graphite/polyimide composites
  - Kevlar/epoxy composites
  - Silica/phenolic composites
  - Selected aluminum alloys
  - Selected titanium alloys
  - Selected stainless steels
  - Selected infrared detector/sensor materials
  - Selected e-m transparent materials
  - Selected thin films

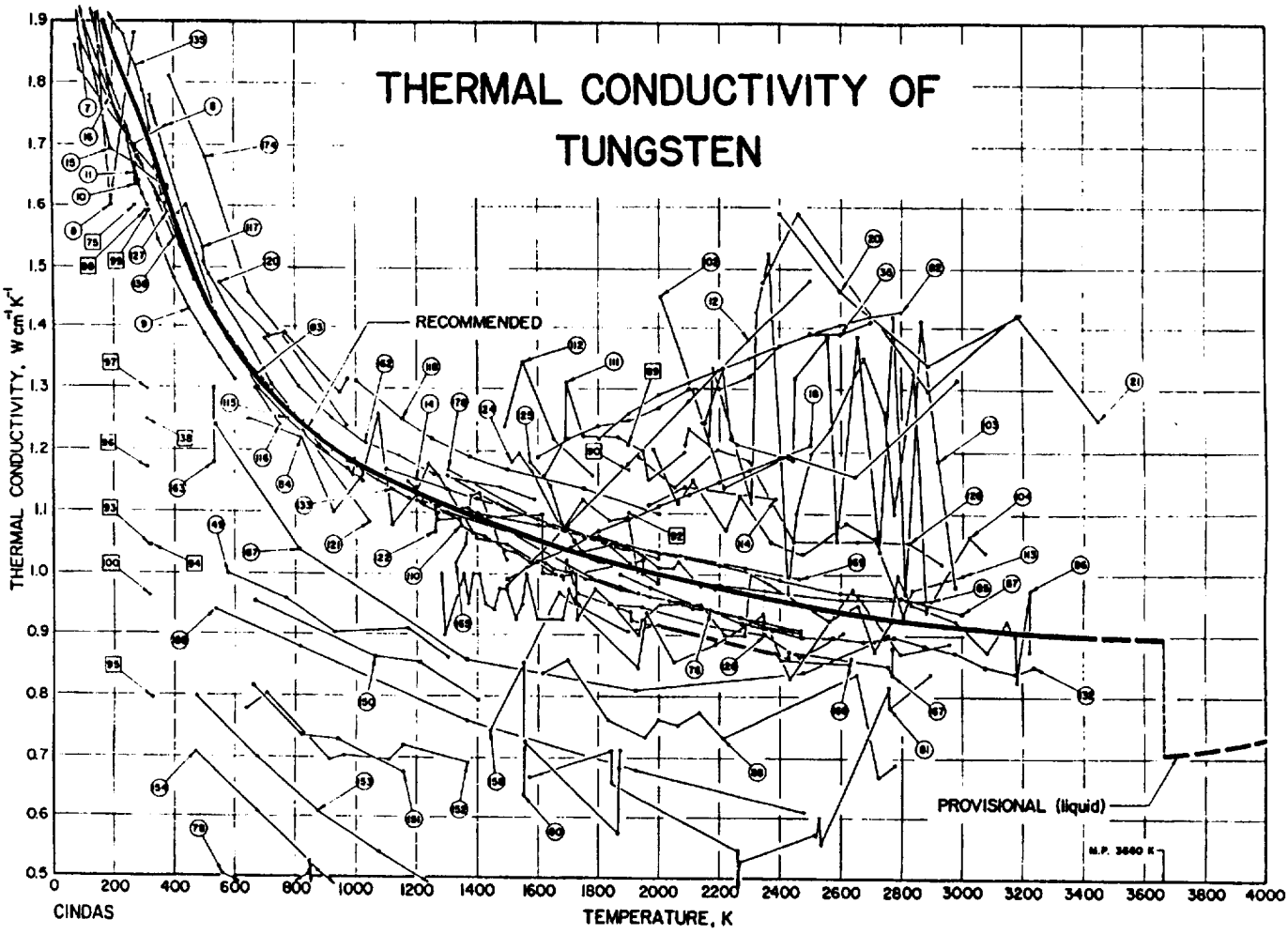
HIGH TEMPERATURE MATERIALS PROPERTIES DATABASE

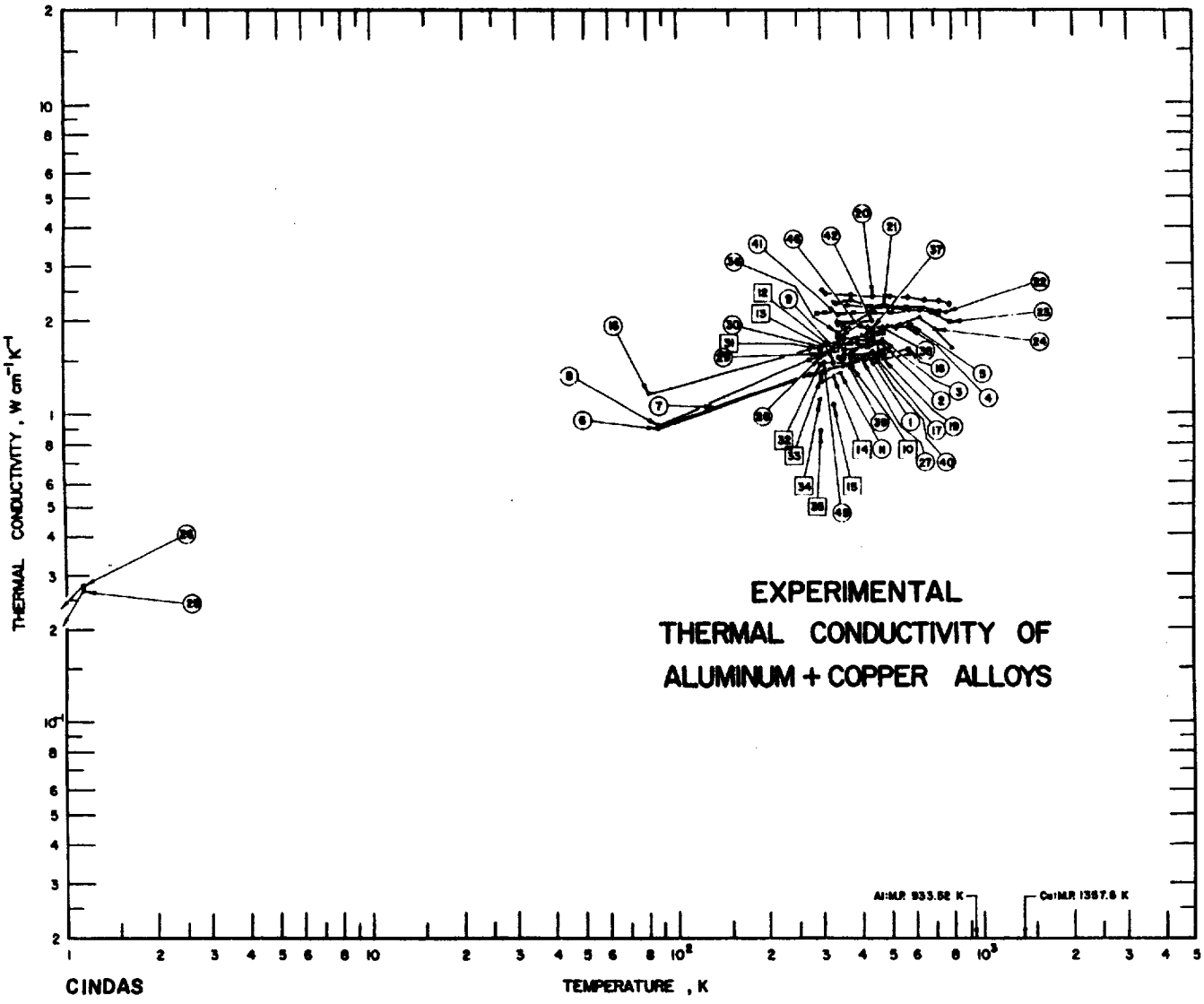
* This is a computerized, online, numerical database
* Contains 21,798 Sets of Data as of 31 December 1991 Covering 720 Materials, 231 Properties, 342 Parameters, and 108 Independent Variables
* Property Groups Covered:
  - Thermophysical properties
  - Thermoradiative properties
  - Mechanical properties
  - Optical properties
  - Electronic properties
  - Ablation properties
  - Physical properties

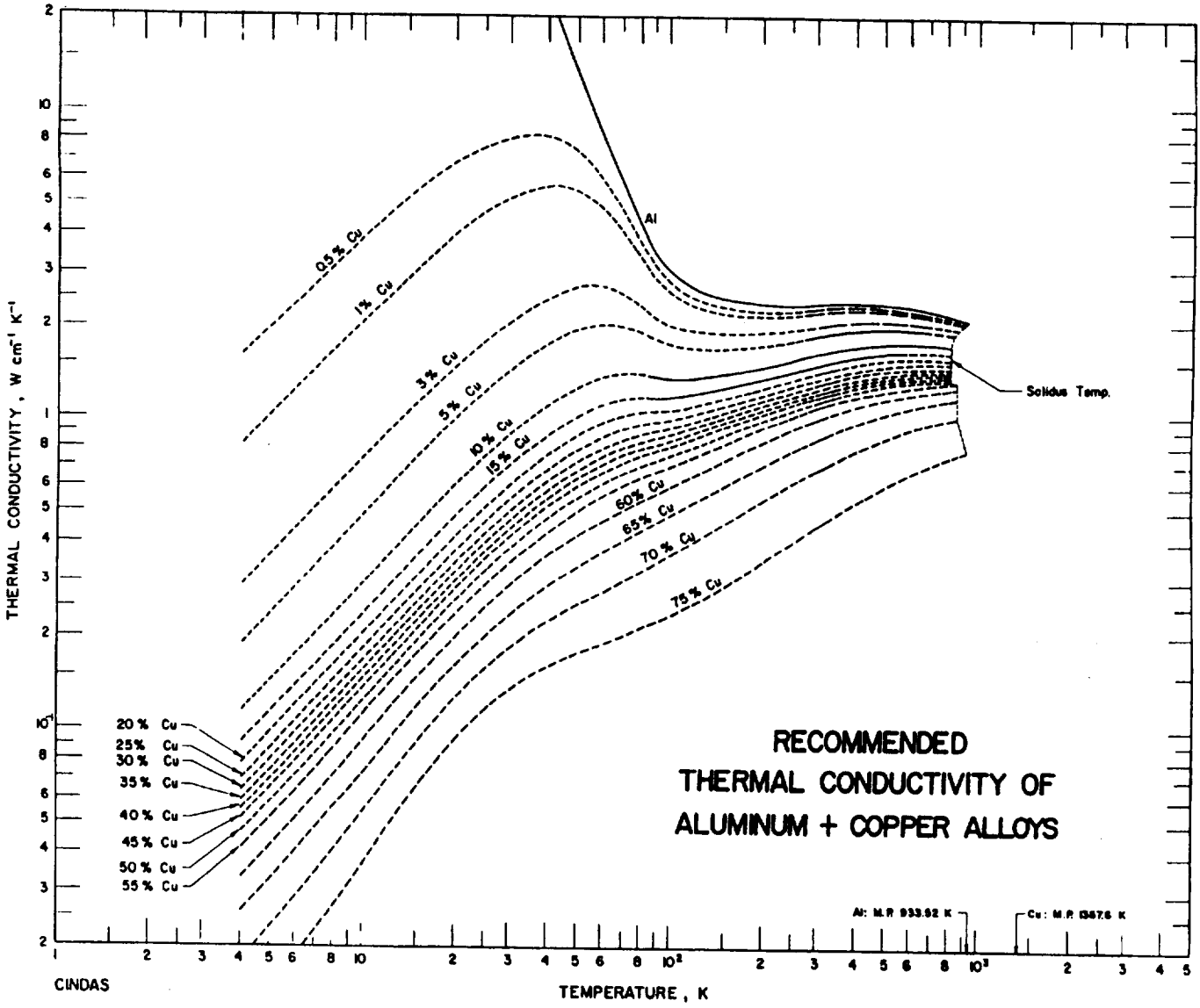
EXAMPLES OF DATA COMPILED AND EVALUATED BY CINDAS

* Thermal Conductivity of Metals in the Solid and Molten States


THERMAL CONDUCTIVITY OF
TITANIUM CARBIDE
THERMAL CONDUCTIVITY , W cm⁻¹ K⁻¹
0.0
0.2
0.4
0.6
500
1000
1500
2000
CINDAS
TEMPERATURE , K
RECOMMENDED
λe
1
2
3
4
5
6
7


THERMAL CONDUCTIVITY OF
TUNGSTEN
THERMAL CONDUCTIVITY, W cm⁻¹ K⁻¹
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4
1.5
1.6
1.7
1.8
1.9
0
200
400
600
800
1000
1200
1400
1600
1800
2000
2200
2400
2600
2800
3000
3200
3400
3600
3800
4000
CINDAS
TEMPERATURE, K
RECOMMENDED
PROVISIONAL (liquid)
M.P. 3660 K


THERMAL CONDUCTIVITY , W cm⁻¹ K⁻¹
TEMPERATURE , K
CINDAS
EXPERIMENTAL
THERMAL CONDUCTIVITY OF
ALUMINUM + COPPER ALLOYS
Al MP 933.52 K
Cu MP 1357.6 K


THERMAL CONDUCTIVITY , W cm⁻¹ K⁻¹
TEMPERATURE , K
CINDAS
Al
Solidus Temp.
0.5 % Cu
1% Cu
3% Cu
5% Cu
10 % Cu
15 % Cu
60% Cu
65 % Cu
70 % Cu
75 % Cu
20 % Cu
25% Cu
30 % Cu
35 % Cu
40 % Cu
45 % Cu
50 % Cu
55 % Cu
RECOMMENDED
THERMAL CONDUCTIVITY OF
ALUMINUM + COPPER ALLOYS
Al: M.P 933.52 K
Cu: M.P 1357.6 K

EXAMPLES OF DATA COMPILED AND EVALUATED BY CINDAS

* Viscosity of Stainless Steels

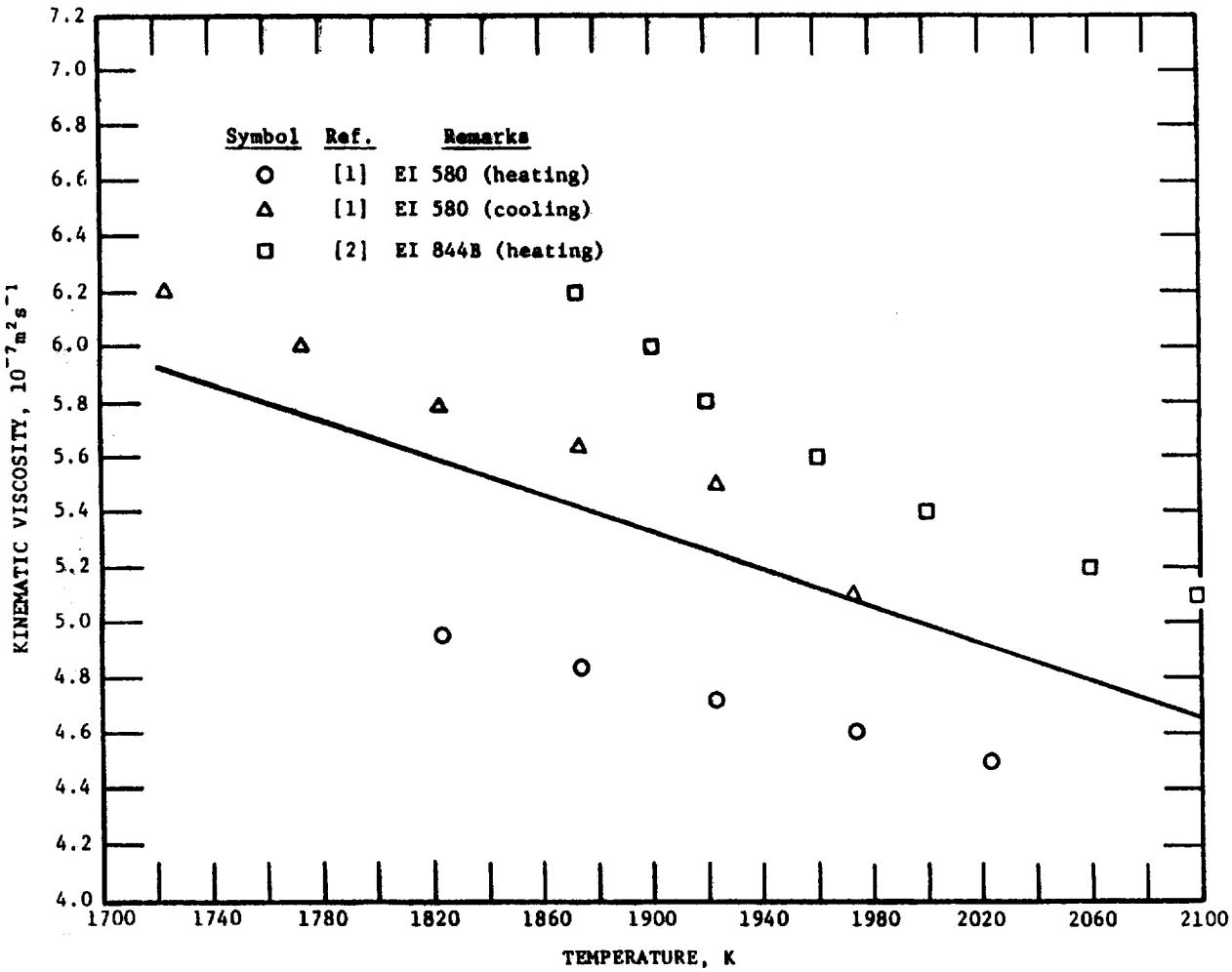


FIGURE 2.12.10. KINEMATIC VISCOSITY OF AISI 316 STAINLESS STEEL.

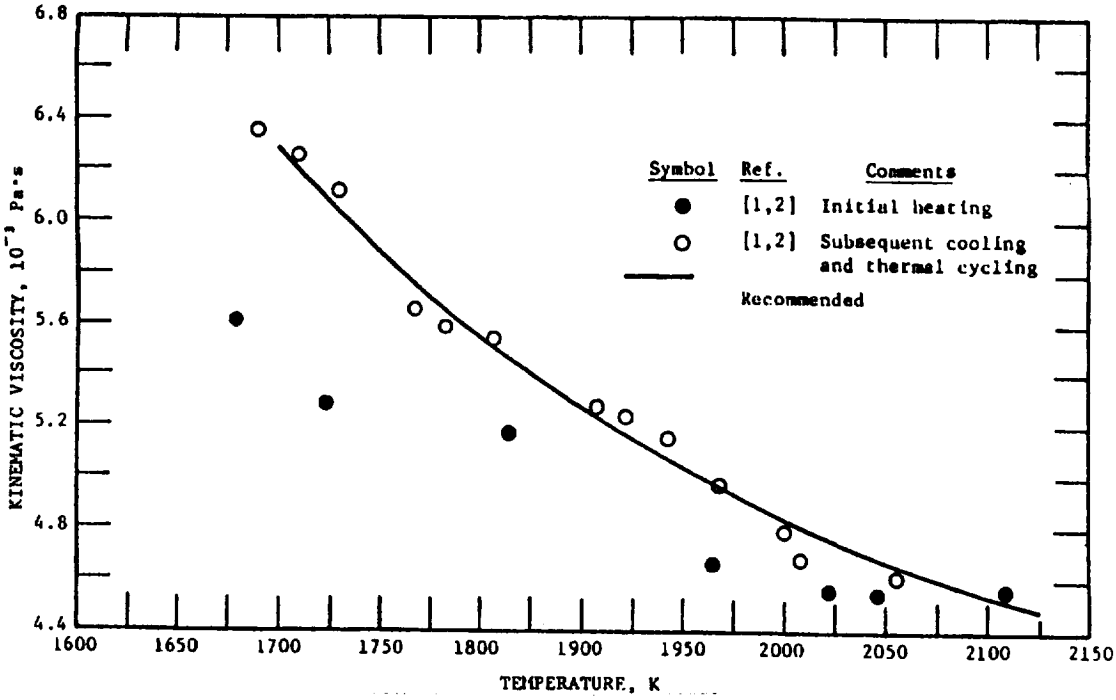


FIGURE 2.14.10. KINEMATIC VISCOSITY OF AISI 321 STAINLESS STEEL.

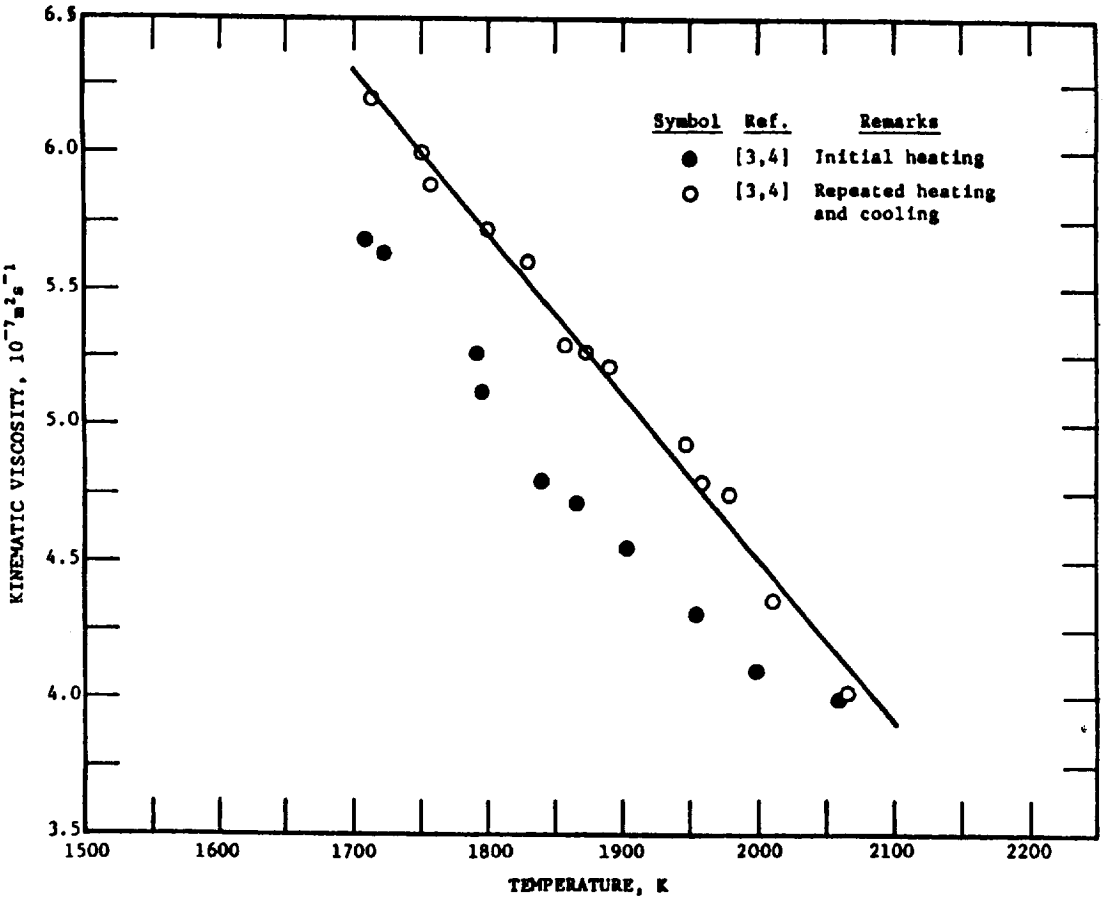


FIGURE 3.5.8. KINEMATIC VISCOSITY OF AISI 446 STAINLESS STEEL.

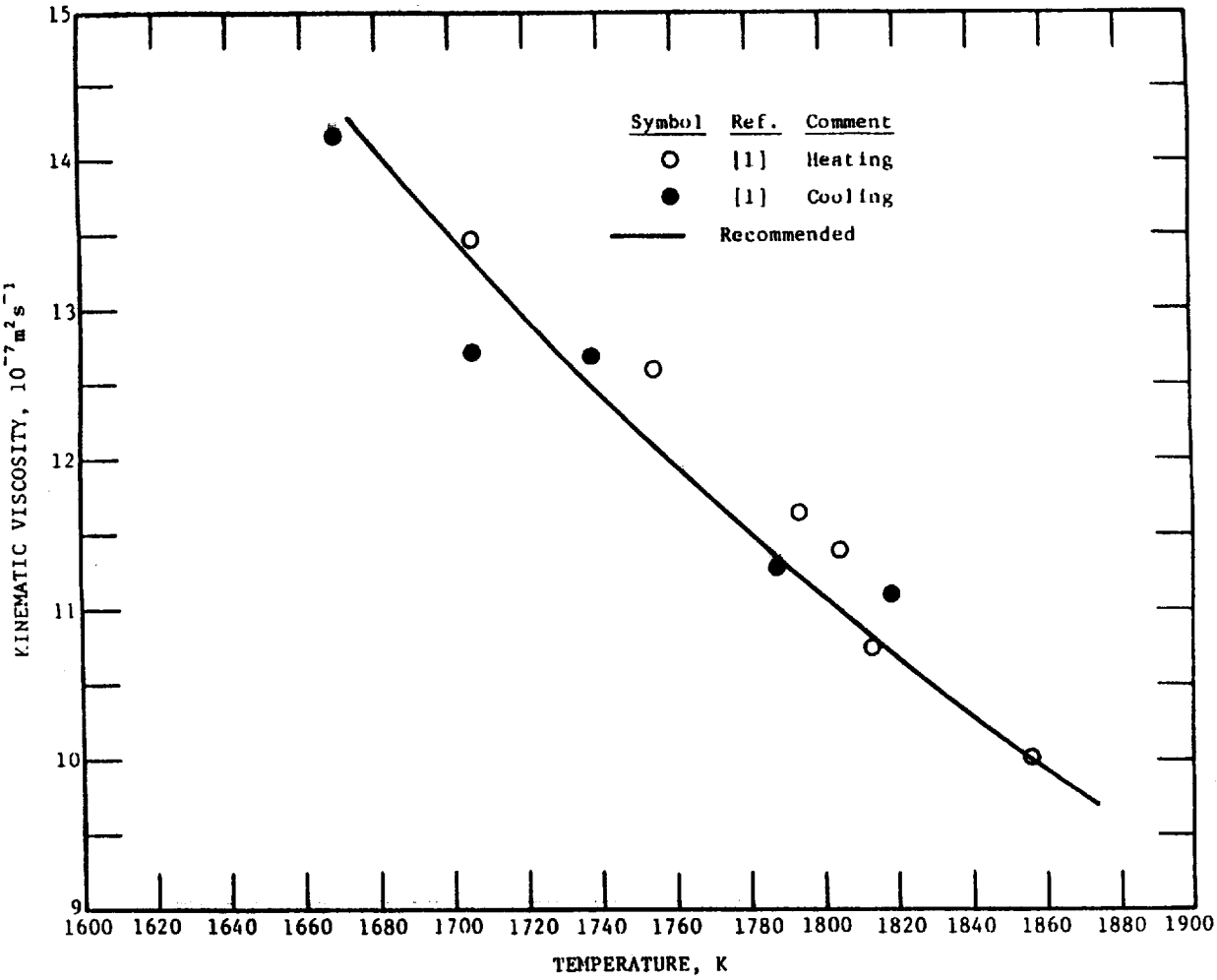


FIGURE 2.22.4. KINEMATIC VISCOSITY OF AISI 660 STAINLESS STEEL [A-286].

Session II

Experimental Techniques