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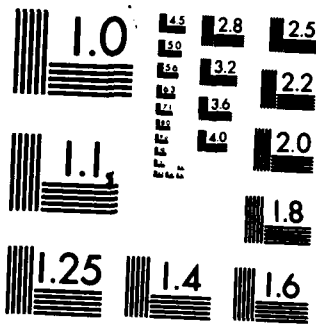
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CODER'S MANUAL

(A Guide to TEPIAC Documentation)

CINDAS REPORT 43.

July 1977

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**CENTER FOR INFORMATION AND
NUMERICAL DATA ANALYSIS AND SYNTHESIS**

CODER'S MANUAL
(A Guide to TEPIAC Documentation)

CINDAS REPORT 43.

July 1977

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PREFACE

TEPIAC's documentation activities involve the collection of recorded information on the thermophysical and electronic properties of matter. TEPIAC has devised a substance classification scheme in which materials are divided into different series and classes according to their chemical and/or physical properties and application. The classification system is a key to the world literature on thermophysical and electronic properties.

This manual provides the rules and definitions of TEPIAC's classification procedure. All amendments in format, definitions, nomenclature rules, etc., which are presented in this manual supersede the contents of the previous editions.

Special thanks are due to a number of CINDAS staff. M. James revised the technical sections on Thermophysical and Electronic Properties. Dr. P. D. Desai, Dr. P. E. Liley, and Dr. R. A. Matula provided useful comments and Mr. H. K. Koutoujian prepared the complete section on the Electronic Properties. Mrs. C. Rodriguez prepared the many tables and proofed the final manuscript.

This manual could not have been written without the advice and assistance of Mrs. J. K. Gerritsen and Mr. J. F. Chaney.

July 1977

V. Ramdas
Editor

INTRODUCTION

One of the major objectives of TEPIAC is to collect recorded information on the thermophysical and electronic properties of matter. The "Retrieval Guide" is a unique publication providing the scientist and engineer with a convenient source of information on thermophysical and electronic properties.

The activities of the Coding Section are involved primarily with the preparation of the directory of substances and the technical coding. This manual should be read thoroughly before the new coder attempts to use TEPIAC's classification system. It will be of maximum value if it is studied in conjunction with the actual substance dictionaries being prepared for the current volume.

The rules set forth in this manual are the key to consistent technical coding. The maintenance of a uniform classification system cannot be overemphasized. It is important, therefore, that any change in TEPIAC's coding policy, however minor, be directly written into this manual to facilitate the preparation of a future edition.

PART I

THE SUBSTANCE CLASSIFICATION SYSTEM AND CODING FORMAT

Thermophysical and electronic properties information at TEPIAC is organized by substance. The classification scheme can accommodate any material for which information about these properties exists or may be generated in the future.

TEPIAC has a classification scheme which is designed to accommodate materials into similar groups, selected preferably by their chemical composition. However, certain substances do not readily lend themselves to a purely chemical classification; they are classified, instead, by their physical form and/or application.

On the following pages the various codes and substance classification criteria are fully discussed:

A. TECHNICAL CODING IN BRIEF

The process of technical coding involves the following steps:

1. Thorough review of the document.
2. Extraction of pertinent information from the document.
3. Translation of the information into code letters (see Part I-B below) recording of the code letters, substance number, and document number on the TEPIAC "Technical Coding Form" (see Part I-C, page 6).
4. Assignment of a substance number and preparation of the substance entry for the materials directory.

After these steps have been completed, the coded information is processed by computer for storage, retrieval, and eventual publication of the "Retrieval Guide."

B. THE CODE LETTERS

The letter codes representing the extracted information from research documents are defined in Tables 1 and 2, page 3 and 4, respectively. Most of the parameters listed in the tables are self-explanatory. Those which require comments are:

1. TEPIAC Properties - A review of the properties can be found in Appendix I and II.
Thermophysical Properties - page 50.
Electronic Properties - page 84.
2. Physical State - Enter separate code lines (multiple coding) if more than one code is needed. Multiple coding is not used (solid not coded) for amorphous solid, superconductive solid, doped solid, expanded solid, fibrous solid, powder solid, or solid film.

- C - Superconductive (superconductive state at temperature $<24^{\circ}\text{K}$)
- D - Doped (impurities intentionally added)
- E - Expanded (including foamed)
- F - Fibrous (or Whisker)
- G - Gas
- I - Ionized (only gases at high temperatures, i. e., Plasmas)
- L - Liquid (including liquid crystals)
- M - Multiphase (powder-fluid, solid-fluid, liquid-gas systems; including suspensoids and emulsions such as petrolatum, blood, paint, mud, paste, gel, etc.)
- P - Powder (loose or cold pressed; including coarser, granular particles)
- S - Solid (including sintered)
- T - Thin or Thick film (A solid thin film will be coded as T only)

3. Dopant - The intentionally added impurity will be identified by the periodic table groups (Table 3, page 5). The appropriate code number for the dopant will be entered in column 15 of the Technical Coding Form (Table 4, page 7).

4. Subject - Write separate code lines (multiple coding) if more than one code is needed.

D - Data (original property values) - No matter how these are obtained or what else is discussed in the paper. Includes data sheets from manufacturers.

E - Experimental - Includes a description, discussion, or theory about the experimental technique or apparatus for the determination of property values.

G - General - Data with experiment and theory.

S - Survey or Review (critical or informative - on a broad scale about experimental techniques or theories). Includes Data Collections (compilation of data on a broad or limited scale, e. g., handbooks, data books, etc.), Discussions and Nomographs. (This does not include papers which contain only one or two values, from literature, for the TEPIAC properties.)

T - Theoretical - Original theory or a modification of an existing theory. A theoretical discussion. Analytical development for the prediction of results.

5. Language - Original foreign language papers and their English translations are assigned separate accession numbers. Such a pair of papers is coded identically, although the appropriate language code letters are used.

- | | | |
|-------------|--------------|-------------|
| C - Czech | G - German | P - Polish |
| D - Dutch | I - Italian | R - Russian |
| E - English | J - Japanese | S - Spanish |
| F - French | O - Other | |

6. Temperature Range - Enter separate code lines (multiple code lines) when there is an overlap of temperature ranges. The code letter N for Normal will be assigned when the temperature is not indicated in the paper.

F - Full range (Low + Normal + High)

L - Low ($\leq -198^{\circ}\text{C}$, $\leq 75^{\circ}\text{K}$, $\leq -324^{\circ}\text{F}$, $\leq 136^{\circ}\text{R}$)

N - Normal ($\leq 1000^{\circ}\text{C}$, $\leq 1273^{\circ}\text{K}$, $\leq 1832^{\circ}\text{F}$, $\leq 2292^{\circ}\text{R}$, or when unspecified)

H - High ($> 1000^{\circ}\text{C}$, $> 1273^{\circ}\text{K}$, $> 1832^{\circ}\text{F}$, $> 2292^{\circ}\text{R}$)

TABLE 1. CODE PARAMETER LETTERS AND NUMBERS OF THERMOPHYSICAL PROPERTIES

| Thermophysical Property | Physical State | Dopant Groups | Subject Coverage | Language | Temperature Range |
|-------------------------------|----------------------------|------------------------------------|-----------------------------|-------------|--|
| A- Thermal Conductivity | C- Super-conductive | 1-IA & IB | D-Data | C- Czech | F- Low + Normal + High |
| B- Accommodation Coefficient | D-Doped | 2-IIA, IIB | E- Experiment | D- Dutch | L- ≤ -198 C ≤ 75 K ≤ -324 F ≤ 136 R |
| C- Thermal Contact Resistance | E- Expanded | 3-IIIA | Theory G- + Expt. + Data | E- English | N- ≤ 1000 C ≤ 1273 K ≤ 1832 F ≤ 2292 R or when unspecified |
| D- Thermal Diffusivity | F- Fibrous or Whisker | 4-IVA | S- Survey, Review | F- French | H- > 1000 C > 1273 K > 1832 F > 2292 R |
| E- Specific Heat | G- Gas | 5-VA | T- Theory | G- German | |
| F- Viscosity | I- Ionized (Plasma) | 6-VIA | | I- Italian | |
| G- Emissivity | L- Liquid | 7-VIIA, VIIB | | J- Japanese | |
| H- Reflectivity | M- Multi-phase | IVB, VB, 8-VIB, VIIB, VIII | | O- Other | |
| I- Absorptivity | P- Powder or Fine Particle | III B, Lanthanide, Actinide Series | | P- Polish | |
| J- Transmissivity | S- Solid | 0- Other or Unspecified | | R- Russian | |
| K- α/ϵ | T- Thin or Thick Film | | | S- Spanish | |
| L- Prandtl Number | | | | | |
| N- Thermal Linear Expansion | | | | | |
| O- Volumetric Expansion | | | | | |

Abstract

A - Coded from abstract
D - Coded from document
H - Hard copy
M - Microfiche

TABLE 2. CODE PARAMETER LETTERS AND NUMBERS OF ELECTRONIC PROPERTIES

| Electronic Property | Physical State | Dopant Groups | Subject Coverage | Language | Temperature Range |
|-----------------------------|----------------------------------|--|--------------------------------|-------------|---|
| AS- Absorption Coefficient | | 1- IA, IB | D-Data | C- Czech | Low + F- Normal + High |
| DC- Dielectric Constant | C- Super- conductive | 2- IIA, IIB | E- Experi- ment | D- Dutch | L- ≤ -198 C ≤ 75 K ≤ -324 F ≤ 136 R |
| DS- Dielectric Strength | D- Doped | 3- IIIA | Theory G- + Expt. + Data | E- English | N- ≤ 1000 C ≤ 1273 K ≤ 1832 F ≤ 2292 R or when unspecified |
| | E- Expanded | | | | |
| EB- Energy Band | F- Fibrous or Whisker | 4- IVA | S- Survey, Review | F- French | |
| EF- Effective Mass | G- Gas | 5- VA | T- Theory | G- German | H- > 1000 C > 1273 K > 1832 F > 2292 R |
| EG- Energy Gap | I- Ionized (Plasma) | 6- VIA | | I - Italian | |
| EH- Electric Hysteresis | L- Liquid | 7- VIIA, VIIIA | | J- Japanese | |
| EL- Energy Level | M- Multiphase | IVB, VB, 8- VIB, VIIB, VIII | | O- Other | |
| ER- Electrical Resistivity | P- Powder or Fine Particle | IIIB, Lanthanide, Actinide Series | | P- Polish | |
| HC- Hall Coefficient | S- Solid | 0- Other or Unspecified | | R- Russian | |
| MH- Magnetic Hysteresis | T- Thin or Thick Film | | | S- Spanish | |
| MO- Mobility | | | | | |
| MS- Magnetic Susceptibility | | | | | |
| RI- Refractive Index | | | | | |
| WF- Work Function | | | | | |

| General Properties | Abstract |
|----------------------------------|---|
| EP- Electron Emission Properties | A- Coded from abstract |
| GP- Magnetoelectric Properties | D- Coded from document H- Hard copy M- Microfiche |
| LP- Luminescence Properties | |
| MP- Magnetomechanical Properties | |
| PP- Photoelectronic Properties | |
| TP- Thermoelectric Properties | |
| ZP- Piezoelectric Properties | |

1D DOPANT
IA GROUP

| | | | |
|----|----|----|----|
| 1 | H | 2 | He |
| 3 | Li | 4 | Be |
| 11 | Na | 12 | Mg |
| 19 | K | 20 | Ca |
| 37 | Rb | 38 | Sr |
| 55 | Cs | 56 | Ba |
| 87 | Fr | 88 | Ra |

MOST ①
METALLIC ②

GUIDE TO DETERMINE WHICH ELEMENT IS CONSIDERED MORE METALLIC.

Naming and order of symbols from more metallic, 1, to more nonmetallic, 26.

EXCEPTIONS: COMMON USAGE

| | | | | | | | | | | | | | | | |
|--|--|-------------------------|-----|--------------------|-----|----------------|-----|-------------|-----|---------|-----|---------------|-----|-----------|-----|
| | | NONMETALLIC | | | | | | | | | | MOST METALLIC | | VIII A | |
| | | 3D IIIA IVA VA VIA VIIA | | 4D IVA VA VIA VIIA | | 5D VA VIA VIIA | | 6D VIA VIIA | | 7D VIIA | | 8D VIII A | | 9D VIII A | |
| | | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 |
| | | B | C | N | O | F | Ne | | | Al | Si | P | S | Cl | Ar |
| | | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 |
| | | Al | Si | P | S | Cl | Ar | Ga | Ge | As | Se | Br | Kr | Xe | Rn |
| | | 31 | 32 | 33 | 34 | 35 | 36 | 37 | 38 | 39 | 40 | 41 | 42 | 43 | 44 |
| | | Ga | Ge | As | Se | Br | Kr | In | Sn | Sb | Te | I | Xe | Rn | |
| | | 49 | 50 | 51 | 52 | 53 | 54 | 55 | 56 | 57 | 58 | 59 | 60 | 61 | 62 |
| | | In | Sn | Sb | Te | I | Xe | Pb | Bi | Po | At | Rn | | | |
| | | 81 | 82 | 83 | 84 | 85 | 86 | 87 | 88 | 89 | 90 | 91 | 92 | 93 | 94 |
| | | Tl | Pb | Bi | Po | At | Rn | Hg | Au | Pt | Ir | Os | Ru | Rh | Pd |
| | | 113 | 114 | 115 | 116 | 117 | 118 | 119 | 120 | 121 | 122 | 123 | 124 | 125 | 126 |
| | | Bi | Po | At | Rn | | | Hg | Au | Pt | Ir | Os | Ru | Rh | Pd |
| | | 81 | 82 | 83 | 84 | 85 | 86 | 87 | 88 | 89 | 90 | 91 | 92 | 93 | 94 |
| | | Tl | Pb | Bi | Po | At | Rn | Hg | Au | Pt | Ir | Os | Ru | Rh | Pd |
| | | 113 | 114 | 115 | 116 | 117 | 118 | 119 | 120 | 121 | 122 | 123 | 124 | 125 | 126 |
| | | Bi | Po | At | Rn | | | Hg | Au | Pt | Ir | Os | Ru | Rh | Pd |

LANTHANIDE SERIES

| | | | | | | | | | | | | | | |
|----|----|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|
| 57 | 58 | 59 | 60 | 61 | 62 | 63 | 64 | 65 | 66 | 67 | 68 | 69 | 70 | 71 |
| La | Ce | Pr | Nd | Pm | Sm | Eu | Gd | Tb | Dy | Ho | Er | Tm | Yb | Lu |
| 89 | 90 | 91 | 92 | 93 | 94 | 95 | 96 | 97 | 98 | 99 | 100 | 101 | 102 | 103 |
| Ac | Th | Pa | U | Np | Pu | Am | Cm | Bk | Cf | Es | Fm | Md | No | Lw |

ACTINIDE SERIES

TABLE 3. PERIODIC TABLE

7. Coding from Abstract

- a. For Thermophysical Properties, only the letter A is used in column 35 to indicate a document coded from abstract. Extended these abstracts and abstracts of articles in translated Russian journals fall under this category.
- b. For Electronic Properties, the following code letters are used in column 35.
 - A = Coded from abstract
 - *H - Hard copy
 - *M - Microfiche.

C. THE TECHNICAL CODING FORM

Code parameter letters, substance classification numbers, and document numbers are written in the appropriate spaces on the Substance Coding Form. On the sample form that follows, Table 4, page 7, "X's" are marked in the spaces which are identified on the right-hand side of the form.

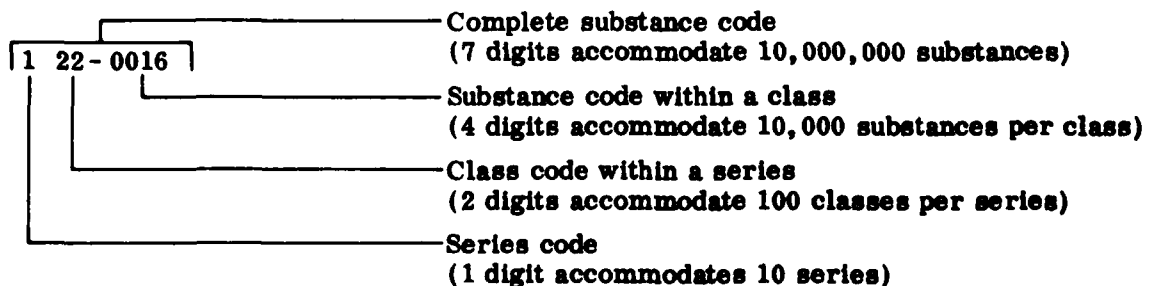
On the lower half of the form a sample paper is coded. A brief description of paper number T69004 (E100961) follows:

"Single-crystal Raman and infrared spectra of vanadium pentoxide." The oriented single-crystal Raman and IR spectra of V_2O_5 were determined, and absorption frequencies were compared with those calculated by using a simple transferred force field. Departures from previously established oxide-group frequencies were due to the relative lightness of V.

D. THE SUBSTANCE CLASSIFICATION NUMBER

Substances are described in one of two forms, i.e., composition, and/or name. Each substance is then assigned a numerical code for processing by computer.

The substance classification code used by TEPIAC has a simple structure. Substances are grouped within 10 series: Each series contains up to 100 classes; and each class contains up to 10,000 substances. Thus the complete arrangement of the series-class-substance code grouping for the seven digit substance number cited in the example on the next page is as follows:



*These codes are for internal use only.

The first three digits of the seven-digit substance code are used as a unit, simultaneously designating both series and class. Thus the range of class numbers within each of the 10 series is: 000 to 099, 100 to 199, 200 to 299, . . . up to 900 to 999.

Presently, seven series (0 to 6) are used, Series 7, 8, and 9 being saved for future expansion.

E. ARRANGEMENT OF THE DIRECTORY OF SUBSTANCES

A summary of the series and classes comprising the Directory of Substances is found in Table 5, page 9.

The Directory of Substances is arranged alphabetically by name (with the exception of certain classes). However, for TEPIAC's internal use the Directory of Substances is arranged by alphabetized formula wherever possible. When the formula or exact composition of the material is unknown, a descriptive name is used. The specific arrangement of the entries is included later in this section with the series and class descriptions.

The lack of well-defined boundaries between certain classes or even series may at times create a difference in outlook between TEPIAC's staff and other users of the "Retrieval Guide". In such a case, it is recommended that the coder consult the present entries of these classes for all possible alternative names before deciding whether a new substance entry is necessary. The Dictionary of Synonyms and Trade Names (see Appendix IV, page 141) should be consulted before determining the substance name for a new entry.

1. Choice of a Class for General or Nonspecific Substances

Series 1 through 5 each has a class or portion of a class which accommodates substances that cannot be identified by a specific substance name. Thus, Classes 100, 200, 300, and 400 are general classes within their respective series. Class 511 (513) accommodates the general or partly identifiable mixtures within Series 5.

If a choice must be made between two such classes, the substance is entered into the most specific class possible; for example, an alloy which is known to be ferrous, but has no exact composition stated, would be entered in Class 300 (Ferrous Alloys).

If it is impossible to decide between two general classes because it is not known whether the substance does or does not fill a certain class qualification, TEPIAC presumes it does not. The substance is then listed in one class only instead of both. For example:

If it is not known whether an alloy is ferrous, it will be entered in Class 400 (Non-Ferrous Alloys).

or

If it is not known whether a solution has water as a solvent or not, it is presumed it does not and it is coded as a nonaqueous mixture.

TABLE 5. A SUMMARY OF THE SERIES AND CLASSES

| | |
|------------------|---|
| SERIES 0 | GENERAL WORKS (Surveys, Handbooks, Apparatus, etc.) |
| SERIES 1 | CHEMICAL ELEMENTS AND COMPOUNDS WHICH DO NOT CONTAIN CARBON AND ANY ISOTOPE OF HYDROGEN (H, D, T) SIMULTANEOUSLY |
| Class 100 | Nonspecific and general compounds and elements, crystals, semi-conductors, etc. |
| Class 101 to 127 | Elements and compounds (primarily inorganic) |
| Class 135 | Intermetallics |
| SERIES 2 | CHEMICAL COMPOUNDS WHICH SIMULTANEOUSLY CONTAIN CARBON AND ANY ISOTOPE OF HYDROGEN (H, D, T) |
| Class 200 | Nonspecific and general compounds: hydrocarbons, ketones, etc. |
| Class 201 to 234 | Compounds (primarily organic) |
| SERIES 3 | FERROUS ALLOYS |
| Class 300 | Nonspecific, general, and unidentifiable alloys |
| Class 304 to 398 | Fe + Al + X to Fe + Zr + X: by predominant alloying constituent |
| SERIES 4 | NONFERROUS ALLOYS |
| Class 400 | Nonspecific, general, and unidentifiable alloys, metallic semiconductors, superconductors |
| Class 402 to 482 | Ac + X to Zr + X: by predominant alloying constituent |
| SERIES 5 | COMBINATIONS OF CHEMICAL COMPOUNDS AND/OR ELEMENTS |
| Class 503 | Oxide mixtures: slags, scales, ceramics, glasses |
| Class 511 | Mixtures and solutions |
| Class 513 | Mixtures and solutions |
| Class 520 | Mixtures designated only by code or trade name |
| Class 521 | Minerals and celestial bodies |
| Class 526 | Aggregate mixes |
| Class 535 | Systems |
| Class 545 | Composites |
| Class 551 | Applied coatings |
| Class 561 | Cermets and mixtures of metals with oxides, carbides, borides, silicides, or nitrides |
| SERIES 6 | NATURAL AND PROCESSED PRODUCTS |
| Class 601 | Pharmaceuticals, cosmetics, toiletries |
| Class 606 | Petroleum base fuels, lubricants, and hydraulic fluids |
| Class 611 | Animal and vegetable natural substances and their derivatives |
| Class 621 | Fabrics, yarns, hairs (woven or processed goods) |
| Class 631 | Rubber, latex, plastics (homogeneous), resins (synthetic), polymers |
| Class 651 | Bulk surface finishes, coatings, inks, adhesives |
| Class 661 | Processed composites, paper and wood products, and building structures |
| Class 671 | Residues |

2. Commercial Designations

A trade name is listed as a substance entry when the generic name of the substance is unknown. If the generic name is known, the substance is entered as a separate entry in the appropriate class, under the generic name followed by the words "commercial designation".

All trade names will be recorded in the "Synonyms Index," see Appendix IV, page 141.

For certain materials there will be individual substance entries to classify selected brand names. These materials will be mentioned under their respective class descriptions.

3. List of Descriptors in the Directory of Substances

| | | |
|-----------------------------|----------------------------------|----------------------|
| adsorbed on | (commercial designations) | insulating |
| animal names, | (company names) | (Latin names) |
| i. e. (bovine, etc.) | (country names, --Russian, etc.) | methylated |
| bounded by | crumpled | natural |
| cast | dyed | nonstoichiometric |
| chlorinated | (general) | (numbered series) |
| clear | glazed | (plastic brand name) |
| colored | human | siliconized |
| (colors - red, white, etc.) | hydroxylated | vulcanized |

The addition of new descriptors must be held to a minimum.

4. Description of the Individual Series and Classes

In this section the substance classification is further discussed, with emphasis on special considerations concerning individual series and classes.

Series 0--General Works

As the title implies, Series 0 locates information that is relevant to substances that cannot be described by one specific name because of the very general or theoretical nature of the research document. These works include theoretical papers, reviews, and descriptions of apparatus and experimental methods.

Class 000 accommodates supplementary general information which can be applied to substances belonging to the other series. Reference works on theory, experimental apparatus, etc., pertaining to specific types of substances are coded under the particular substance numbers in their proper series and class.

The entries in this class do not represent substance names in the true sense of this word. Hence, the "pseudosubstance" numbers merely represent concepts such as black body, semi-infinite medium, groove, surface, etc. Also included are entries such as: Experimental technique, Handbook, Survey, Theory.

Series 1-- Chemical Elements and Compounds Which Do Not Contain Carbon and Any Isotope of Hydrogen (H, D, T) Simultaneously

Substances are classified in Series 1 if their chemical formulas do not contain carbon (C) and either hydrogen (H), deuterium (D), or tritium (T) simultaneously; for example, AgBr, H₂SO₄, CBrCl₃, etc.

Chemical elements and compounds are indexed alphabetically by name. They are listed by alphabetized formula for in-house use only. Molecular formulas are included on substance entries to aid in the identification of compounds. The rules for the writing of molecular formulas and for general nomenclature are discussed in Part III, page 41.

Individual class descriptions for Series 1 are as follows:

Class 100 -- Nonspecific

Class 100 includes general material names with no specific formula which chemically belong to any one of the classes in either Series 1 or 2. Examples are Barium compound; Element, metallic; Liquid, thixotropic; Crystal, ferromagnetic; etc.

Class 101 -- Elements and Their Isotopes

Table 6 contains a list of chemical element names and symbols.

1. Allotropy--Allotropy is disregarded except in the case of carbon. Graphite and carbon receive separate entries; natural diamond is coded as a gem in Class 521, and charcoal is in Class 671 as a residue.

Separate substance entries will be made for the various commercial and special types of graphite. The commercial graphites will be listed in categories arranged alphabetically. For example, Graphite CEP will be listed under Graphite, C series; Graphite L-56 under Graphite, L series; etc.

There will be separate substance numbers for the following graphites:

| | |
|---------------------|---------------------------|
| Graphite, AG series | Graphite, numbered series |
| Graphite, AT series | Graphite, pyrolytic |
| Graphite, AX series | Graphite, Ceylon |

2. Impurities--TEPIAC defines the "impurity" limits of an element as follows: When each individual impurity is < 0.2 weight percent and the total amount of impurities is < 0.5 weight percent, the substance is considered an element.

TABLE 6. CHEMICAL ELEMENT NAMES AND SYMBOLS

| | | | | | |
|-----|----------------------------|-----|---------------------|-----|----------------------------|
| Ac | Actinium | *He | Helium | Pm | Promethium |
| Ag | Silver | Hf | Hafnium | | (Illinium, Il) |
| Al | Aluminum | | (Celtium, Ct) | Po | Polonium |
| Am | Americium | Hg | Mercury | Pr | Praseodymium |
| *Ar | Argon | | (Hydrargyrum) | Pt | Platinum |
| | (also A) | Ho | Holmium | Pu | Plutonium |
| *As | Arsenic | *I | Iodine | Ra | Radium |
| *At | Astatine | | (Jodium, J) | Rb | Rubidium |
| | (Alabamine, Ab) | In | Indium | Re | Rhenium |
| Au | Gold | Ir | Iridium | Rh | Rhodium |
| *B | Boron | K | Potassium | *Rn | Radon |
| Ba | Barium | | (Kalium) | | (Actinon, |
| Be | Beryllium | *Kr | Krypton | | Niton) |
| | (Glucinium, Gl) | Ku | Kurchatovium | Ru | Ruthenium |
| Bi | Bismuth | | (Rutherfordium, Rf) | *S | Sulfur |
| Bk | Berkelium | La | Lanthanum | Sb | Antimony |
| *Br | Bromine | Li | Lithium | | (Stibium) |
| *C | Carbon | Lr | Lawrencium | Sc | Scandium |
| Ca | Calcium | | (also Lw) | *Se | Selenium |
| Cd | Cadmium | Lu | Lutetium | *Si | Silicon |
| Ce | Cerium | | (Cassiopeium) | Sm | Samarium |
| Cf | Californium | Md | Mendelevium | | (also Sa) |
| *Cl | Chlorine | | (also Mv) | Sn | Tin |
| Cm | Curium | Mg | Magnesium | Sr | Strontium |
| Co | Cobalt | Mn | Manganese | *T | Tritium |
| Cr | Chromium | Mo | Molybdenum | | (heavy H, H ³) |
| Cs | Cesium | *N | Nitrogen | Ta | Tantalum |
| Cu | Copper | Na | Sodium | Tb | Terbium |
| | (heavy H, H ²) | | (Natrium) | Tc | Technetium |
| Dy | Dysprosium | Nb | Niobium | *Te | Tellurium |
| Er | Erbium | | (Columbium, Cb) | Th | Thorium |
| Es | Einsteinium | Nd | Neodymium | Ti | Titanium |
| | (also E) | *Ne | Neon | Tl | Thallium |
| Eu | Europium | Ni | Nickel | Tm | Thulium |
| *F | Fluorine | No | Nobelium | U | Uranium |
| Fe | Iron | Np | Neptunium | V | Vanadium |
| Fm | Fermium | *O | Oxygen | W | Tungsten |
| Fr | Francium | Os | Osmium | | (Wolfram) |
| Ga | Gallium | *P | Phosphorus | *Xe | Xenon |
| Gd | Gadolinium | Pa | Protactinium | Y | Yttrium |
| Ge | Germanium | Pb | Lead | | (also Yt) |
| *H | Hydrogen | | (Plumbum) | Yb | Ytterbium |
| | | Pd | Palladium | Zn | Zinc |
| | | | | Zr | Zirconium |

* The starred elements are considered as nonmetallic elements by TEPIAC. When more than one name or symbol is indicated for an element, TEPIAC uses the name and associated symbol listed first.

A metal having an individual impurity ≥ 0.2 weight percent and total impurities ≥ 0.5 weight percent, is considered an alloy. A nonmetal having an individual impurity ≥ 0.2 weight percent and total impurities ≥ 0.5 weight percent is considered a mixture. See Chemical Element Notations, page 12, for those elements considered metallic by TEPIAC. (TEPIAC follows the International Line in the Periodic Table separating Metallic and Nonmetallic elements.)

The impurity limits for a compound are: When each impurity is < 2.0 weight percent, and the total amount of impurities is < 5.0 weight percent, the substance is considered to be a pure compound.

A compound having impurities in excess of these limits is considered a mixture.

(Note: An intermetallic compound having a (i) metallic impurity in excess of these limits is listed as an alloy in Series 3 and 4; (ii) nonmetallic impurity above these limits is considered a mixture.)

3. Doping--TEPIAC defines "doping" as impurity(ies) intentionally added. The physical state code letter "D" indicates a doped substance (generally a solid). However, if the substance is a liquid (or gas) and is also doped, then 2 entries are made on the code sheet to indicate a liquid (or gas) and a doped material.

The dopant will be identified by the periodic table groups (Table 3, page 5), and the dopant number entered in column 15 of the Technical Coding Form.

4. Dilute Alloys--If the weight percent composition for a so-called "dilute alloy" cannot be identified, TEPIAC presumes the quantity of impurities added to the major metallic element is below the impurity limit (No. 2 above); therefore, the alloy is listed in Class 101 as a doped element (No. 3 above).
5. Natural Isotopes of Hydrogen and Helium--An isotope is listed under the corresponding element as a single entry. Exceptions are the isotopes of hydrogen (deuterium and tritium) and helium (helium 3 and helium 4) which are listed separately from their respective element of natural isotopic abundance. A compound of isotopic elements is treated in the same manner. The forms of helium 4, He-I and He-II, are not listed separately from the He4 entry.

The elements D_2 and T_2 are listed as "Deuterium" and "Tritium." TEPIAC names deuterium and tritium compounds as the corresponding hydrogen compound with a descriptive term indicating the number of deuterium or tritium atoms. Examples are DH = hydrogen,

monodeuterated (DH is listed as a compound); T_2S = hydrogen sulfide, ditritiated; etc.

6. Adsorbed Gases and Liquids-- For the property specific heat, gases or liquids adsorbed on substrates are entered in Series 1 or 2 as "gas (or liquid), adsorbed on surface," for example, Argon, adsorbed on nickel.

Class 102 through 135 -- Compounds (Primarily Inorganic)

1. Class Format-- The first letter of the alphabetized formula determines the class. Table 7, page 15, contains a summary of the alphabetical letters assigned to classes 102 through 135. Listed also are some sample entries.

In these classes, each substance entry contains an alphabetized formula, molecular formula, and a chemical name for the compound. An example is given below:

| <u>Alphabetized Formula</u> | <u>Molecular Formula</u> | <u>Substance Name</u> |
|-----------------------------|--------------------------|-------------------------|
| AgS ₂ Sb | AgSbS ₂ | Antimony silver sulfide |

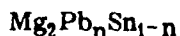
2. Nonstoichiometric Compounds-- The word "nonstoichiometric" will follow the compound name. The numerical subscripts in the formula will be expressed in whole numbers and/or letters. See Part III-A, page 41, for a complete description.
3. Metallic Compounds-- A compound consisting of metallic elements only is listed in Class 135 as an intermetallic. (See below.)

Class 135 -- Intermetallics

TEPLAC has defined an "intermetallic" as a simple stoichiometric composition consisting of metallic elements only.*

Examples of intermetallics are $MnPt_3$, $Cd_2Sb_5Zn_3$. For entries in this class the names of the elements are listed alphabetically followed by the word "intermetallic". The elements in the intermetallic formula are also arranged alphabetically. See Table 8, page 16, for some sample formats.

The formula for an intermetallic, the composition of which can be expressed as a range, is written as:



* If an author has not identified a metal-metal combination, the only way to verify that it is an intermetallic would be to consult phase diagrams. Since this research task could be very time-consuming, metal-metal mixtures are arbitrarily identified as intermetallics if they are of stoichiometric composition.

TABLE 7. SUMMARY OF CLASSES IN SERIES 1 AND SERIES 2

| Class | Alphabetical Letter | Sample Entries* | Class | Alphabetical Letter | Sample Entries* |
|-------|---------------------|---|-------|---------------------|---|
| 100 | Nonspecific | | 200 | Nonspecific | |
| 101 | Elements | | 201 | CH compounds only | CH ₄ |
| 102 | A | AgCl ₂ | 203 | A | C ₃ H ₉ Al [Al(CH ₃) ₃] |
| 104 | B | BN | 204 | B | CHBr ₃ |
| 106 | C | CCaO ₃ [CaCO ₃] | 206 | C | CHCl ₃ |
| 108 | D | D ₂ O | 208 | D | CH ₂ D ₂ |
| 109 | E | Er ₂ O ₃ | 209 | E | C ₆ H ₁₅ ErO ₁₂ S ₃ [Er(C ₂ H ₅ SO ₄) ₃] |
| 110 | F | F ₂ Fe [FeF ₂] | 210 | F | CH ₃ F |
| 111 | G | GaO ₄ P [GaPO ₄] | 212 | G | C ₈ H ₂₀ Ge [Ge(C ₂ H ₅) ₄] |
| 112 | H | HNO ₃ | 213 | H | C ₁₂ H ₁₀ Hg [(C ₆ H ₅) ₂ Hg] |
| 114 | I | INa [NaI] | 214 | I | CH ₃ I |
| 116 | K | K ₂ O ₄ S [K ₂ SO ₄] | 216 | K | C ₂ H ₃ KO ₂ [CH ₃ COOK] |
| 118 | L | LiO ₃ Ta [LiTaO ₃] | 217 | L | C ₆ H ₁₅ LaO ₁₂ S ₃ [La(C ₂ H ₅ SO ₄) ₃] |
| 119 | M | MnO ₃ Si [MnSiO ₃] | 218 | M | C ₂ H ₂ MnO ₄ [(HCOO) ₂ Mn] |
| 120 | N | NNaO ₃ [NaNO ₃] | 219 | N | CHN [HCN] |
| 122 | O | O ₄ SiZr [ZrSiO ₄] | 221 | O | CH ₂ O [HCHO] |
| 123 | P | PbS | 223 | P | CH ₃ P |
| 125 | R | RbS ₂ Sb [RbSbS ₂] | 226 | S | CH ₄ S [CH ₃ SH] |
| 126 | S | S ₃ Sb ₂ [Sb ₂ S ₃] | 227 | T | CHT ₃ |
| 127 | T | TZn [ZnT] | 232 | Y | C ₁₅ H ₁₅ Yb [Yb(C ₅ H ₅) ₃] |
| 135 | Intermetallics | MnPt ₃ | 234 | | CD ₄ ; CCl ₂ DT [CDTCl ₂] |

* Formulas are alphabetized, with molecular formulas in brackets (wherever applicable).

A metal combined with an intermetallic is listed as an alloy in Series 3 and 4. A nonmetal combined with an intermetallic is considered a mixture.

TABLE 8. A SAMPLE FORMAT FOR CLASS 135 - INTERMETALLICS

| | | |
|----------|---------------------------------------|--------------------|
| 135-1230 | Aluminum Molybdenum Intermetallic | $AlMo_3$ |
| 135-1232 | Aluminum Molybdenum Intermetallic | Al_2Mo |
| 135-4233 | Aluminum Nickel Niobium Intermetallic | $Al_nNb_{1-n}Ni_3$ |
| 135-1234 | Bismuth Lead Tin Intermetallic | Bi_6Pb_2Sn |
| 135-1235 | Lead Magnesium Tin Intermetallic | $Mg_2Pb_nSn_{1-n}$ |

* Series 2 -- Chemical Compounds Which Simultaneously Contain Carbon and Any Isotope of Hydrogen (H, D, T)

Substances are classified in Series 2 if their chemical formulas contain C and H (or any of its isotopes) simultaneously; for example, $CHCl_3$, C_2H_5OH , CD_4 , etc. As with Series 1, Series 2 compounds are classified on the basis of alphabetized formula, for internal use only. For publication, the substances are listed alphabetically by chemical name, followed by molecular formulas.

A description of the classes follows:

Class 200 -- Nonspecific

The entries in this class are of a general nature. The lead words for these compounds are their functional names, such as acid, alcohol, amine, ester, hydrocarbon, ketone, silicate, etc. The main subdivisions of qualifying names which follow these lead words are:

1. aliphatic (alkane, alkene, or alkyne)
2. alkyaromatic
3. aromatic

Examples of the entries in Class 200 are:

Hydrocarbon, aliphatic, alkane, halogenated;
Ether, cyclic, fluorinated

* Electronic Properties are excluded for Series 2 at present.

The terms "saturated" and "unsaturated" are preferred to "hydrogenated" and "dehydrogenated", respectively. Paraffin hydrocarbons are listed as "Hydrocarbon, aliphatic, alkane."

Classes 201 through 232-- Compounds (Primarily Organic)

1. Class Format

The alphabetical letter that represents each of these classes corresponds to the element symbol occurring after "CH" in the alphabetized formula (see Table 7, page 15). The rules and examples of writing formulas and nomenclature for Series 2 are discussed in Part III, page 41.

Class 234--Class 234 contains hydrocarbon compounds which are completely deuterated and/or tritiated. Examples are: CD_2Cl_2 , CD_3F .

Series 3 and 4 -- The Alloy Series

These series contain mixtures of metal-metal or metal-nonmetal components in which the metal is greater than 50 weight percent. (If the nonmetal portion is greater than 50 weight percent, then the substance is listed in Class 511 (513) as a mixture. An alloy having an equal amount of metal and nonmetal components is entered as an alloy as well as a mixture.)

The alloys are classified according to weight percent composition. Every class in these series represents a major alloying element.

Series 3 -- Ferrous Alloys

A ferrous alloy is one in which iron, Fe, is the principal constituent ($Fe \geq$ any other single element). One class is assigned to each primary element alloying with Fe. The arrangement order within classes is covered in the discussion of classification criteria. The specific classes in Series 3 are described below.

Class 300 -- Nonspecific

The ferrous alloys listed here are either general or ones for which TEPIAC cannot identify the composition; for example, Iron alloy; Steel, stainless; Russian steel 20.

Classes 304 through 398 -- Specific Classes

These classes are assigned alphabetically according to the predominant constituent element other than Fe. See Table 9, page 18, for a summary of the classes.

TABLE 9. SUMMARY OF THE CLASSES IN SERIES 3 AND 4

| Class | Description | Class | Description | Class | Description |
|-------|--------------|-------|-------------|-------|-------------|
| 300 | Nonspecific | 400 | Nonspecific | 442 | Nb + X** |
| 304 | Fe + Al + Q* | 401 | Ac + X** | 443 | Nd + X |
| 306 | Fe + As + Q | 402 | Ag + X | 444 | Ni + X |
| 307 | Fe + Au + Q | 403 | Al + X | 445 | No + X |
| 308 | Fe + B + Q | 405 | Au + X | 446 | Np + X |
| 310 | Fe + Be + Q | 407 | Be + X | 447 | Os + X |
| 313 | Fe + C + Q | 408 | Bi + X | 448 | Pa + X |
| 317 | Fe + Ce + Q | 409 | Ba + X | 449 | Pb + X |
| 320 | Fe + Co + Q | 410 | Ca + X | 450 | Pd + X |
| 322 | Fe + Cr + Q | 411 | Cd + X | 451 | Pm + X |
| 328 | Fe + Cu + Q | 412 | Ce + X | 452 | Po + X |
| 333 | Fe + Ga + Q | 413 | Cf + X | 453 | Pr + X |
| 334 | Fe + Gd + Q | 414 | Cm + X | 454 | Pt + X |
| 335 | Fe + Ge + Q | 415 | Co + X | 455 | Pu + X |
| 336 | Fe + Hf + Q | 416 | Cr + X | 456 | Ra + X |
| 339 | Fe + In + Q | 417 | Cs + X | 457 | Rb + X |
| 340 | Fe + Ir + Q | 418 | Cu + X | 458 | Re + X |
| 342 | Fe + La + Q | 419 | Dy + X | 459 | Rh + X |
| 343 | Fe + Lu + Q | 420 | Er + X | 460 | Ru + X |
| 344 | Fe + Mg + Q | 421 | Es + X | 461 | Sm + X |
| 345 | Fe + Mn + Q | 422 | Eu + X | 462 | Sb + X |
| 348 | Fe + Mo + Q | 423 | Fm + X | 463 | Sc + X |
| 350 | Fe + N + Q | 424 | Fr + X | 466 | Sn + X |
| 352 | Fe + Nb + Q | 425 | Ga + X | 467 | Sr + X |
| 353 | Fe + Nd + Q | 426 | Gd + X | 468 | Ta + X |
| 355 | Fe + Ni + Q | 427 | Ge + X | 469 | Tb + X |
| 359 | Fe + O + Q | 428 | Hf + X | 470 | Tc + X |
| 360 | Fe + Os + Q | 429 | Hg + X | 472 | Th + X |
| 361 | Fe + P + Q | 430 | Ho + X | 473 | Ti + X |
| 362 | Fe + Pb + Q | 431 | In + X | 474 | Tl + X |
| 363 | Fe + Pd + Q | 432 | Ir + X | 475 | Tm + X |
| 365 | Fe + Pt + Q | 433 | K + X | 476 | U + X |
| 368 | Fe + Re + Q | 434 | La + X | 477 | V + X |
| 369 | Fe + Rh + Q | 435 | Li + X | 478 | W + X |
| 370 | Fe + Ru + Q | 436 | Lu + X | 479 | Y + X |
| 372 | Fe + Sb + Q | 437 | Md + X | 480 | Yb + X |
| 374 | Fe + Si + Q | 438 | Mg + X | 481 | Zn + X |
| 378 | Fe + Sn + Q | 439 | Mn + X | 482 | Zr + X |
| 381 | Fe + Tb + Q | 440 | Mo + X | | |
| 384 | Fe + Tl + Q | 441 | Na + X | | |
| 390 | Fe + V + Q | | | | |
| 392 | Fe + W + Q | | | | |
| 394 | Fe + Y + Q | | | | |
| 397 | Fe + Zn + Q | | | | |
| 398 | Fe + Zr + Q | | | | |

* Q represents the next 2 major constituents in descending weight order plus carbon.

** X represents the next 4 major constituents in descending weight order.

Series 4 -- Nonferrous Alloys

A nonferrous alloy is one in which a metallic element other than iron is the principal constituent.

Descriptions of individual classes in Series 4 follow:

Class 400 -- Nonspecific

General alloys and alloys known by name only, which TEPIAC cannot identify as ferrous or nonferrous are listed here. Examples are: Alloy, Semiconductor, APM-M257, etc.

Class 401 through 482 -- Specific Classes

These classes are assigned alphabetically according to the predominant element. See Table 9, page 18, for a summary of the classes.

Classification Criteria for Series 3 and 4

1. Impurity criteria--A metal containing ≥ 0.5 percent total impurities or ≥ 0.2 percent individual impurity, is considered an alloy.

When each impurity is < 0.2 weight percent and the total impurities are < 0.5 weight percent, the substance is classified as an element.

For example $\left[\begin{array}{cccccc} \text{Fe} & + & \text{C} & + & \text{B} & + & \text{Si} & + & \text{Ti} \\ 99.6\% & & 0.1\% & & 0.1\% & & 0.1\% & & 0.1\% \end{array} \right]$ is entered in Class 101 as IRON.

When each impurity is < 0.2 weight percent and the total impurities are ≥ 0.5 weight percent, the substance is classified as an alloy of the base metal.

For example $\left[\begin{array}{ccccccccc} \text{Fe} & + & \text{B} & + & \text{P} & + & \text{Si} & + & \text{Ti} & + & \text{W} & + & \text{V} \\ 99.4\% & & 0.1\% & & 0.1\% & & 0.1\% & & 0.1\% & & 0.1\% & & 0.1\% \end{array} \right]$
(≥ 0.5 weight percent)

entered in Class 300 as IRON ALLOY, 99.4 PERCENT.

2. Significant Figures

Weight percents will be rounded off to the nearest whole number, or if less than .95, to the nearest tenth, i. e., 29.65 is listed as 30, 0.56 is listed as 0.6, etc.

3. Substance Entries

A maximum of 5 components will be listed for each alloy. The entries will be arranged by composition in decreasing weight percent.

Brand name alloys and experimental alloys will have separate entries. Brand names are written to the right of the composition. In Tables 10 and 11, pages 20 and 21, are shown some sample formats for alloys in Series 3 and 4.

TABLE 10. A SAMPLE FORMAT FOR FERROUS ALLOYS

Series 3 - Ferrous Alloys, Class 322 (Fe + Cr + X)Commercial Alloys

| | | |
|----------|-------------------------------------|-----------|
| 322-0164 | 55 Fe + 24 Cr + 15 Ni + 2 Mn + .2 C | *AISI-309 |
| 322-0123 | 51 Fe + 25 Cr + 21 Ni + 2 Mn + .3 C | *AISI-310 |
| 322-0225 | 67 Fe + 26 Cr + 5 Ni + 2 Mo + .2 C | *AISI-329 |

Experimental Alloys

| | |
|----------|---------------------------------------|
| 322-0953 | 0- 76 Fe + 0- 74 Cr + 24- 26 Be |
| 322-7327 | 0-100 Fe + 0-100 Cr |
| 322-0722 | 10- 90 Fe + 4- 85 Cr + 5 Al |
| 322-7632 | 20- 80 Fe + 10- 40 Cr + 10- 40 Ni |
| 322-7326 | 98 Fe + .8 Cr + .6 Si + .2 Mn + .1 C |
| 322-0979 | 95 Fe + 1 Cr + 1 Si + 1 Mn + .4 C |
| 322-0289 | 82 Fe + 14 Cr + 2 Si + 1 Mn + .4 C |
| 322-4236 | 60 Fe + 25 Cr + 13 Al + 2 Si + .4 Mn |
| 322-1240 | 62 Fe + 25 Cr + 13 Ni + .2 Si |
| 322-1241 | 52 Fe + 25 Cr + 20 Ni + 2 Si + .7 Mn |
| 322-1101 | 74 Fe + 25 Cr + .6 Si + .3 Mn |
| 322-1238 | 71 Fe + 28 Cr + .5 Mn + .4 Si + .2 C |
| 322-1239 | 71 Fe + 28 Cr + .5 Mn + .4 Si + .2 Ni |
| 322-2237 | 70 Fe + 29 Cr + .6 Mn + .4 Si |
| 322-1235 | 70 Fe + 30 Cr |
| 322-1234 | 60 Fe + 40 Cr |

TABLE 11. A SAMPLE FORMAT FOR NONFERROUS ALLOYS

Series 4 - Nonferrous Alloys, Class 444 (Ni + X)Commercial Alloys

| | | |
|----------|-------------------------------------|-------------|
| 444-0089 | 95 Ni + 2 Al + 2 Mn + 1 Si | *Alumel |
| 444-0101 | 54 Ni + 20 Cr + 18 Co + 5 Fe + 2 Ti | *Nimonic 90 |

Experimental Alloys

| | |
|-----------|--------------------------------------|
| 444-0697 | 0-100 Ni + 0-100 Al |
| 444-0996 | 0- 95 Ni + 5-100 Al |
| 444-0994 | 44- 75 Ni + 20- 52 Cu + 5 Al |
| 444-1234 | 69 Ni + 31 Al |
| †444-1235 | 30 Ni + 20 Co + 20 Cr + 20 Fe + 3 Mo |
| 444-1236 | 71 Ni + 10 Cr + 6 Al + 6 W + 3 Mo |
| 444-1239 | 73 Ni + 10 Cr + 6 W + 4 Al + 3 Mo |
| 444-1237 | 73 Ni + 19 Cr + 7 Mo + .3 Si |
| †444-1235 | 30 Ni + 20 Cr + 20 Co + 20 Fe + 3 Mo |
| 444-1238 | 65 Ni + 30 Cr + 7 Ti + 2 Al + .4 Mn |
| †444-1235 | 30 Ni + 20 Fe + 20 Co + 20 Cr + 3 Mo |

† The alloy 30 Ni + 20 Co + 20 Cr + 20 Fe + 3 Mo has multiple entries (with the same substance number), since the three major elements alloying with nickel are of equal weight percent.

4. Composition of the Alloys

- a. **Commercial Alloys** - A reference handbook composition is used whenever an alloy has been referred to by its trade name or symbol. Handbook nominal compositions are noted by an asterisk preceding the alloy's name.

When the composition of an alloy is given as a range, the average of the upper and lower limits will be used. The average will be rounded off to the nearest whole number, or if less than .95, to the nearest tenth. If the composition is listed as a minimum (or a maximum) then the minimum (or maximum) value will be used.

In calculating the balance, all separate weight percents should not be rounded off prior to the calculation.

A list of alloy handbooks is included in the bibliography (Appendix III, page 140). The primary reference sources are the Engineering Alloys and Metals Handbook. AISI is always the preferred specification. SAE, ASTM, UNS, and other designations are given as cross-references to AISI in the Synonyms Index.

- b. **Experimental Alloys** - If the composition is given as a range, the upper and lower limits of the range will be listed in the substance entry. There may be entries in more than one class because of the range. For example, 0 to 100 percent Cr alloyed with Fe would be listed in

- (i) Class 322 as a ferrous chromium alloy
- (ii) Class 416 as a chromium alloy
- (iii) Class 101 with Chromium and Iron as pure elements.

Atom or mole percent is converted to weight percent and listed in the appropriate class.

5. Alloys Having Major Constituents With Equal Compositions

- a. **Commercial Alloys** - In a commercial alloy composition, if the 5th and 6th components are of equal weight percent, the first element based on alphabetical order of symbol will be retained.

- b. **Experimental Alloys** - For an experimental alloy, if the 5th and 6th components are of equal weight, 2 entries are made to include the 5th or 6th component, respectively. For example, for an alloy with 73Ni + 10Cr + 6W + 4Al + 3Mo + 3Ti, there will be 2 entries, with different substance numbers, as follows:

(i) 73Ni + 10Cr + 6W + 4Al + 3Mo

(ii) 73Ni + 10Cr + 6W + 4Al + 3Ti.

An alloy with the composition 30Ni + 20Co + 20Cr + 20Fe + 3Mo will have entries as follows:

(i) 30Ni + 20Co + 20Cr + 20Fe + 3Mo

(ii) 30Ni + 20Cr + 20Co + 20Fe + 3Mo

(iii) 30Ni + 20Fe + 20Co + 20Cr + 3Mo.

All three entries will have same substance number. Two of the entries will be cross-referenced to the one assigned the primary substance number.

6. Alloys of Indefinite Composition

An alloy of indefinite or unknown composition is named as precisely as the information of the paper allows. Only one substance

entry is made for each general alloy, even though *some of these* alloys could actually belong to more than one class. Therefore, the following class preferences are given to general alloys:

- a. A general alloy, known to be ferrous, such as stainless steel, austenitic steel, is entered in the ferrous alloy Class 300.
- b. An alloy of totally unknown composition, or one which cannot be identified as a ferrous alloy, is located in Class 400 and given a general name, such as: Alloy, Semiconductor, etc.
- c. Classes in Series 4, other than Class 400, accommodate general entries for which the major alloying element is known. For example Aluminum alloy, Titanium alloy, etc.

7. Commercial Alloys

- a. Commercial alloys with identical compositions but different names or numbers are entered under the previously listed alloy and appropriate entries are made in the Synonyms Index.
- b. If a paper deals with a commercial alloy to which the experimenter has added various elements, this is considered to be an experimental alloy (since it no longer has the same composition as the starting material).

8. Foreign Alloys

Foreign alloy names are preceded by the country of origin; for example, French T-A4D3V, Russian 1Kh18N9T. Foreign and American commercial alloys should be merged only when they have identical compositions. Entries will be made for the American alloy while the foreign alloy will be listed in the Synonyms Index.

9. Dilute Alloys

If a "dilute alloy" of known composition fulfills the impurity criteria of No. 1 above, it is entered in Series 3 or 4 as an alloy. If the weight percent composition for a "dilute alloy" cannot be identified, TEPIAC presumes the quantity of impurities added to the major metallic element is below the impurity limit; therefore, the alloy is listed in Class 101 as a doped element.

10. Doping Elements and Nonspecific Alloying Constituents

Alloys intentionally doped with impurities are so indicated only in the physical state, code letter "D". See No. 3, page 13, for further explanation.

When the amount of one or more alloying elements is not specified, the word contraction "Unsp", denoting unspecified, is used. The term "Sat'd" (contraction for saturated) is also used as an indication of undefined composition.

11. Nonmetallic Elements in Alloys

In some cases, important constituents in an alloy may be non-metallic elements. For example, ferrous alloys accept carbon as an element. For Ferrous Alloys only, if the amount of Carbon is less than 0.2 weight percent, it is rounded off and reported to the nearest tenth (that is 0.05 is listed as 0.1, etc.)

12. Intermetallic compounds with metal impurity(ies) added are listed as alloys. The substance entries follow the format of the alloys.

Series 5 -- Combinations of Chemical Compounds and/or Elements

Series 5 includes combinations of substances that are mixtures, aggregates, systems*, or composites.

Classes 511 (513) contain nonaqueous and aqueous mixtures. The other classes in Series 5 accommodate mixtures of special groups such as oxides, minerals, aggregate mixes, systems, surface coatings, and cermets. These classes will be identified later in this text.

The interrelation between certain classes in Series 5 and Series 6 should be mentioned. Because of the broad scope of content in the Systems Class 535 and Composites Class 545, a more narrowly defined class is provided for certain groups of substances used primarily as common construction materials. Class 661 (Processed Composites, Paper and Wood Products, and Building Structures) serves this purpose.

The coder should be aware of the possibility of entering a substance in the more specialized Class 661, even though it would also fulfill the criteria for the composite class or other materials classes. Three examples follow:

1. Wood, a natural substance, is listed in Class 611; however, plywood, a processed composite of wood, is listed in Class 661.
2. Class 503 contains bricks, but bricks in a special form, wall structures, are located in Class 661.
3. Nylon fabric is entered in Class 621; but a multilayer of nylon and polyamids will be listed in the Systems Class 535. And a resin reinforced with nylon fabric is entered in the Composites Class 545.

The "impurity" limits for an element or a nonmetallic compound have been stated in the Class 101 discussion and are reiterated here. A mixture is constituted when the amount of impurities in an element is ≥ 0.5 weight percent total or ≥ 0.2 weight percent individual impurity. The corresponding limits for a

* For definition of 'system' see page 27.

nonmetallic compound are ≥ 5.0 weight percent and ≥ 2.0 weight percent, respectively. These criteria apply to all the classes in Series 5.

Class 503 -- The Oxide Mixtures (Ceramics, Glasses, and Slags)

Substance Entries - In this class are accommodated slags and scales, ceramics, glasses, etc. composed of oxide mixtures. See Table 12 below.

1. Commercial oxide mixtures--Entries will be made using commercial names. When known, cross-references to experimental oxide mixtures will be made.
2. Experimental oxide mixtures--Entries will indicate the molecular formula for four major oxides in descending weight percent order with the word "other" following if one or more additional oxides are present which are above the impurity limits. The type of mixture will be noted by descriptors following the composition; for example, Ceramic, glass, glaze, porcelain, refractory, scale, brick slag, or oxide mixture. Names such as "Borosilicate glass" will also be used when they are necessary.

The same chemical composition may exist with more than one descriptor. Each entry will carry a separate substance number, for instance:

- a. 503-0010 $\text{SiO}_2 + \text{Al}_2\text{O}_3 + \text{Na}_2\text{O}$ Glass
- b. 503-0011 $\text{SiO}_2 + \text{Al}_2\text{O}_3 + \text{Na}_2\text{O}$ Slag

When the oxide mixture has 2 (or more) components of equal weight percent, there will be 2 (or more) entries. For example, a glass with $\text{SiO}_2 + \text{Al}_2\text{O}_3 + \text{Na}_2\text{O} + \text{CaO} + \text{Other}$, where Al_2O_3 , Na_2O , and CaO are equal in weight, there will be entries as follows:

TABLE 12. A SAMPLE FORMAT FOR CLASS 503 - OXIDE MIXTURES (CERAMICS, GLASSES, AND SLAGS)

| <u>Brand Names:</u> | | |
|---------------------|---|---------------|
| 503-1234 | Corning Glass 9700 | |
| 503-2147 | Enamel 853 (Pfaudler) | |
| 503-1321 | Russian Glass LF (numbered series) | |
| 503-2148 | Schott Glass F | |
| 503-1324 | $\text{SiO}_2 + \text{Al}_2\text{O}_3 + \text{MgO} + \text{CaO} + \text{TiO}_2$ | Ceramic glass |
| 503-2111 | $\text{SiO}_2 + \text{Al}_2\text{O}_3 + \text{MgO} + \text{TiO}_2$ | Ceramic |
| 503-0301 | $\text{SiO}_2 + \text{PbO} + \text{MgO} + \text{BaO}$ | Glass |

- a. 503-0120 $\text{SiO}_2 + \text{Al}_2\text{O}_3 + \text{Na}_2\text{O} + \text{CaO} + \text{Other}$ Glass
 b. 503-0260 $\text{SiO}_2 + \text{Na}_2\text{O} + \text{Al}_2\text{O}_3 + \text{CaO} + \text{Other}$ Glass
 c. 503-0760 $\text{SiO}_2 + \text{CaO} + \text{Al}_2\text{O}_3 + \text{Na}_2\text{O} + \text{Other}$ Glass

Class 511 (513)* -- Mixtures and Solutions (Nonaqueous and Aqueous)

Substance Entries - All entries will be arranged alphabetically. The substance name will be followed by the molecular formula in parentheses. A maximum of the four largest components will be listed. Only one entry will be assigned a substance number. The remaining entries will have cross-references to the one with the substance number.

Aqueous Mixtures - Aqueous mixtures are identified only on the coding form by a mixture code "W" (to indicate Water) in column 13.

Examples of entries in this class are:

Air
 Combustion products of fuel
 Helium (He) + Nitrogen (N_2)
 Chloroform (CHCl_3) + Methane (CH_4)

1. Combustion of rocket fuels with a number of reactants is listed as "Combustion products of rocket fuel."
2. Plasmas (and Arcs) which consist of mixtures of ionized gas particles, usually at high temperatures, are listed in this class.
3. Flames are products of combustion normally containing high percentages of water vapor. Therefore, they are coded as aqueous mixtures with the mixture code "W".
4. Atmospheres of planets are listed in Class 521 (Minerals and Celestial Bodies).
5. Air, Cloud, Dust, Rocket Exhaust, Sea Water, etc. are mixtures by their very nature, and hence listed in this class.
6. Mixtures containing one or more polymers is excluded from coding.

Class 520 -- Mixtures Designated Only by Code or Trade Name

The substances in this class are ones which TEPIAC has not been able to classify. They are listed by their code or trade names. When a substance is identified, it is transferred to its appropriate class with an entry in the Synonyms Index.

*Class 513, an overflow class assigned to Class 511, will be used only when a mixture has not been identified in Class 511.

Examples of entries in this class are: Dowtherm, Orophen AK 50, Polyran M15 N.

Class 521 -- Minerals and Celestial Bodies

Ores, minerals, planets, and soils are listed in this class; synthetic or refined minerals are classified in Series 1 as compounds. Examples of this class are: Garnet; Mars surface; Earth mantle; Coal.

Class 526 -- Aggregate Mixes

An aggregate consists of hard, inert fragments of material mixed with a cementing substance. Examples are: Concrete (cement-gravel); Cement; Plaster; Mortar.

Class 535 -- Systems

A "system" is a combination of materials with clearly defined boundaries existing between them, or a distinct configuration of more than one homogeneous material.

Substance Entries - The components in a system are arranged alphabetically. A system of a general nature may be identified by a lead word, as for instance: Filter, interference; Fuel, nuclear.

A few lead words will be retained to group similar structures or materials. The components following the lead words will be alphabetized. The lead words are:

| | | |
|--------|---------------|------------|
| Adduct | Fluidized bed | Packed bed |
| Cable | Honeycomb | Propellant |
| Coil | Multilayer | Solar cell |

Examples of entries in this class are: Air gap; Fluidized bed, glass beads; Alclad 2024; Copper-Magnesium oxide, etc.

Two thermal properties pertaining to the Systems class are Accommodation Coefficient (Property B) and Thermal Contact Resistance (Property C).

- a. Entries for Accommodation Coefficient are listed as "Gas on solid". For example, Helium on tungsten.
- b. The Thermal Contact Resistance between two materials, listed alphabetically, will be identified only by the property letter "C". If the contact is between two identical materials, for example, two copper surfaces, the entry will be "Copper-Copper".

Certain substances (foils, greases, fluids, etc.) are used to fill the gaps between contact surfaces. Separate entries are made for such contact surfaces, followed by the words "with filler". Example: Aluminum-Copper, with filler.

The following comments apply to this class:

1. Multilayers--All parallel multilayer systems are entered with the lead word "multilayer", with the various components arranged alphabetically. The descriptors for multilayer systems like fibrous, foamed, fabric, etc. are omitted. (Foamed and fibrous systems are indicated in the physical state by the letters E and F, respectively.) The term "sandwich" is synonymous to "multilayer".
2. Air--Air is considered as a systems component when the property measurement is directly concerned with the air itself, as with property B (Accommodation Coefficient). Example: Air on mercury.
3. A system may contain certain components which are composites; for example, a filled honeycomb or a multilayer of reinforced resin. Such materials are included in this class (not in the Composites class 545) since the entire structure is a system.

Class 545 -- Composites

A "composite" is considered to be a combination of materials differing in composition or form on a macroscale. The constituents retain their identities in the composite; that is, they do not dissolve or otherwise merge completely into each other although they act in concert. Normally, the components can be physically identified and exhibit an interface between one another.

Certain composites are accommodated in individual classes: Minerals (Class 521); Aggregate Mixes (Class 526); Cermets (Class 561); Processed Composites and Building Structures (Class 661).

Substance Entries - Entries will list the reinforcement followed by the matrix, the two being separated by a slash. If there are two or more components in the reinforcement, they will be alphabetized and separated by plus signs (+). A reinforcement material may have a coating or covering. This is regarded as a second component; hence, the entry will indicate two components as the reinforcement.

Examples of entries are: Graphite/Epoxy resin.
Carbon + Graphite/Epoxy resin.

The following comments are relevant to the Composites class:

1. Reinforced materials--All reinforced materials are indexed in this class.
2. Filled Polymers--Polymers which have a nonorganic filler (e. g., mica, aluminum oxide) belong to this class.

3. Matrices--A solid filled matrix forms a composite. Such matrices are the filled graphites, glasses, etc.
4. Shape or Form--The various forms of reinforcement, such as fibers, filaments, fabric, etc., are disregarded.

Class 551 -- Applied Coatings

The coatings here are applied on a substrate, and hence differ from the bulk paints, coatings, etc. of Class 651. Radiative properties for the coatings are entered in this class.

Substance Entries - The entry is described by the top coating. However, for multilayer coatings, such as those used for filters, all the components are alphabetically listed. Substrates are ignored in the entries.

Examples of entries in Class 551 are:

Aluminum
Aluminum-magnesium fluoride
Germanium-zinc sulfide, multilayer
Paint (TiO₂ + silicone)
Paint, black Japalac 1208 (Glidden)

1. Paints and Ceramics

a. "Paint" includes all paints, enamel paints and lacquers. Paint compositions are listed with the pigment (usually a metallic oxide) preceding the vehicle or binder, the constituents of which are arranged alphabetically. Paint textures like flat, gloss, satiny, sheen, etc. are ignored.

Example: Paint (TiO₂ + acrylic resin + silicone)

b. "Ceramic" includes all ceramic coatings, glazes, and enamels. Ceramic compositions are listed alphabetically by the four major constituents.

Example: Ceramic (Al₂O₃ + BaO + Cr₂O₃ + SiO₂)

2. Resins

a. Resin is used as a lead word for all polymer coating entries except silicones.

b. "Silicone" includes all substituted silicone resins, such as methyl silicone, etc.

Examples: Resin, polyamide
Paint (Al + silicone)

3. Special Chemical Surface Treatments and Commercial Finishes

a. Chemical surface treatments are used as lead words.

Examples: Anodized aluminum, Oxidized lead, Siliconized graphite, etc.

b. Commercial Finishes are listed by their trade names.

Examples: Armco Process, HAE Finish, Dow Finish, etc.

4. Oxidized Metal vs Metal Oxide

- a. An "oxidized metal" refers to a metal with an oxide surface coating that has been produced by a chemical reaction oxidation process.

Oxidized alloys are described by trade name or number. If the trade name is unknown, the major element alloying with the base metal is noted in the entry.

Examples: Oxidized aluminum
Oxidized Zircaloy 2
Oxidized Copper alloy (Ni)

- b. A "metal oxide" refers to a metal with a metal oxide coating applied as a surface finish, i. e., the oxide coating has not been produced by any chemical reaction with the base metal.

Example: Aluminum oxide

5. Trade Names

- a. The trade name of a coating is not used in a substance entry if its composition is known. It is listed, however, in the Synonyms Index.

- b. A coating identified only by a code symbol should have its manufacturer, when available, listed with it.

- c. The trade name of an alloy coating is used in a substance entry.

Examples: Coating RTV 60 (General Electric)
Inconel X

6. Color -- Color, when it is indicated in the paper, is included with the substance entries. If the pigment in a paint is known, the color is disregarded. Colors are limited to black, blue, brown, green, grey, orange, purple, red, white, yellow.

Class 561 -- Cermets and Mixtures of Metals With Oxides, Carbides, Borides, Silicides, and Nitrides

Cermets are a group of composite materials consisting of an intimate mixture of ceramic and metallic components. Ceramic components may be oxides, carbides, borides, silicides, nitrides, or mixtures of these compounds; the metallic components, which are the bonding agents, are pure metals, alloys, or intermetallic compounds. Cermets are also known as ceramels.

Also included in this class are mixtures which are not chemically bonded.

Substance Entries - The entries are arranged alphabetically, with the ceramic preceding the metallic components. Cermets are so indicated on the substance entry.

Entries in this class are subject to the impurity criteria stated in Series 1 (page 11). An entry is made here when:

In a mixture of a metal and an oxide (or a carbide, boride, silicide, or nitride),

- a. The oxide is between 0.2-98 weight percent (or the metal component is between 2-99.8 weight percent).
- b. An oxide >98 weight percent is listed in Series 1 as a pure oxide.
- c. A metal >99.8 weight percent is listed in Class 101 as a pure element.

Examples are: Silicon oxide - Aluminum cermet
Uranium oxide - Stainless 316 cermet

Series 6 -- Natural and Processed Products

The class titles themselves are quite self-explanatory as to the general content of each class. The substance names are alphabetized within each class.

Class 601 -- Pharmaceuticals, Cosmetics, Toilettries

The substances in this class are determined mainly by their use.

Examples are: Penicillin; Perfume; Tincture, benzoin.

Class 606 -- Petroleum Base Fuels, Lubricants and Hydraulic Fluids

Class 606 includes only petroleum base fluids, greases, fuels, etc. Lead words for entries are primarily indicative of use; for example, Bearing oil, Cylinder oil, Grease, Motor oil, etc., or are general names indicative of source; for example, Coal oil, Mineral oil, Shale oil, etc. A trade name or code symbol is used only if no other designation is available; for example, Dynamo oil, Texaco oil, JP-4 fuel, etc. Since oils are generally not pure, the presence of additives is ignored in the substance entries.

Class 611 -- Animal and Vegetable Natural Substances and Their Derivatives

General lead words are used in this class with a specific common or generic term or trade name as a descriptor. All parts of a plant (or tree) are listed under its specific name, with the exception of the juice and wood which are used as lead words. Only the Latin genus name is listed as a descriptor. The entries in this class also include processed substances (frozen, cooked, crushed, freeze-dried, etc.).

Examples of Class 611 are: Apple (*Malus sp.*); Blubber, seal; Fish, salmon; Juice, orange; Wood, aspen (*Populus sp.*).

Class 621 -- Fabrics, Yarns, Hairs (Woven or Processed Goods)

Examples of the processed goods are: Calico, Cotton fabric, Flannel, Glass fabric, Haircloth, Wool yarn, Nylon fabric, etc.

Fibers (single or bulk) are listed in the class of materials of which they are composed. For example, fiberglass is listed in Class 503; aluminum oxide fiber is listed in Class 102; nylon fiber is in Class 631, etc.

Class 631 -- Rubber, Latex, Plastics (Homogeneous), Resins (Synthetic), Polymers

Substance Entries - Polymer components are listed by name only. The polymers are identified as:

- a. Poly - Polymers produced by the condensation reaction of two or more molecular units.
- b. Copoly - Polymers produced by the addition reaction of two different molecular units.
- c. Terpoly - Polymer produced by the addition reaction of three different molecular units.

(Polymer nomenclature is discussed in Part III, page 45)

Examples of Entries are: Polyethylene
Copoly (acrylonitrile-butadiene)
Terpoly (acrylonitrile-butadiene-styrene)

The following comments apply to this class:

1. Polymers with nonorganic "fillers", such as mica, or aluminum oxide powder, are entered in the Composite Class 545.
Polymers with fillers of an organic nature, such as *Diocetyl adipate*, or wood shavings, or various plasticizers are retained in this class. However, these additives are ignored in the substance entry.
2. Natural and synthetic latexes and rubbers are included in this class.
3. Natural carbohydrates such as cellulose and starch belong to Class 611 (Natural products).
4. Oligomers with a defined degree of polymerization are listed in Series 1 and 2. For example, $(\text{BeCl}_2)_2$ Beryllium chloride, dimeric is in Class 104.
5. Some polymers in this class do not carry the lead word designations "Poly-", "Copoly-", or "Terpoly-". Examples are: Cellulose acetate; Latex, chloroprene; Resin, epoxy; Rubber; Silicone; etc.
6. Polymers are entered under their generic names. A commercial polymer is listed under its generic name followed by the words "Commercial designation ". However, the following commercial polymers will receive separate substance entries, that is, generic name followed by brand name:

| | |
|-----------|--------------|
| Lucite | Silicone RTV |
| Mylar | Teflon |
| Plexiglas | Teflon FEP |

7. For a nonspecific polymer without a trade name, the name of the manufacturer, if indicated in the paper, is used to identify the compound further. For example, Polyethylene glycol compound 20M (Union Carbide).

Class 651 -- Bulk Surface Finishes, Coatings, Inks, Adhesives

The substances in this class are not to be confused with the surface coatings in Class 551. The coatings of this class are in their natural form and are not applied to a base.

Chemical constituents are listed alphabetically by name after the lead word; for example, Lacquer (maleic anhydride-olive oil). A trade name is listed only when chemical composition is not fully known. The trade name should, however, be entered in the Synonyms Index. Color is specified only when the radiative properties are coded.

Examples of lead words and descriptors are: Glue, fish; Ink, printing; Paint, acrylic; Pigment, yellow ochre.

Class 661 -- Processed Composites, Paper and Wood Products, and Building Structures

The physical shape and use of these substances govern the choice of this class. The common construction materials in Class 661 are actually systems and composites, having a specialized use. (See the introduction to Series 5, page 24, for a discussion of the relation of this class to classes 535 and 545.)

Examples of the substance types in Class 661 are Cardboard; Glass fiber blanket; Linoleum; Mineral wool felt; Plywood; Wall, adobe; Air space bounded by glass; Tile (acoustical); Insulation

Class 671 -- Residues

Examples are Petroleum residue; Charcoal; Bone char; Asphalt; Waste, radioactive; Soot; Tar.

PART II
THE PREPARATION OF SUBSTANCE ENTRIES

Substance entries need particular attention before they are added to the TEPIAC Materials Directory. The procedures for preparing correct entries are described below.

Every substance is assigned a class and a unique substance number, which is recorded in the Technical Coding Form (page 7). Before making any entries, the coder should check in the existing Materials Directory whether the substance already has a number. If the substance has been assigned a number, the coder merely records it in the Technical Coding Form. If the substance does not have a number, then the procedure described below should be followed.

A. PREPARATION OF NEW SUBSTANCE ENTRIES

Each coder is allotted a set of 10,000 Temporary Substance Numbers, for example, 900-0000 to 900-9999, where the first three digits indicate the class assigned to the coder. When a substance number cannot be located in the existing Materials Directory, the coder assigns the lowest temporary number in his (her) set to that substance. This temporary substance number is then recorded in the Technical Coding Form and a Temporary Substance Number Form (see below). Each new substance is assigned one temporary number in increasing order until all the numbers are used up. The coder will then be allotted a new set of temporary numbers.

Series 9 has been reserved for temporary substance numbers. Classes 900, 911, 922, 933, and 944 will be used by the coders of Thermophysical Properties, and classes 955, 966, 977, 988 and 999 by the Electronic Properties Coders.

B. THE TEMPORARY SUBSTANCE NUMBER FORM

| Temporary Substance Number | Actual Substance Number* | Substance Name, With and Without Formula | Synonym | Document Number |
|----------------------------|--------------------------|--|---------|--------------------|
| 900-0000 999-0000 | 102-0002 101-0020 | Aluminum Oxide Al_2O_3 Aluminum | Alumina | T 12345 E 67890 |

* Actual Substance Numbers will be assigned by the Editor.

The coder should enter the Temporary Substance Number, Substance Name, any Synonyms for the substance, and the Document Number in the Temporary Substance Number Form. Every two weeks this form is handed to the Editor of the coding section.

The Editor checks the correctness of the substance name (i. e., whether the name is consistent with the TEPIAC naming procedures) and if the substance has a number. If the substance does not have a number, then the Editor assigns an actual, unique number to that substance (the lowest unused number of the class assigned to the substance), and records this substance number in the Temporary Substance Number Form.

C. THE SUBSTANCE CODING FORM

After the substance has been assigned a number, the Editor enters the information (the substance number, the correct name, and any synonyms) in a Substance Coding Form (see Table 13, page 36). This Substance Coding Form contains columns similar to an IBM computer card. The Editor completes this Substance Coding Form, taking into account the formats for the substance entries (below) and the rules for keypunching (page 39). The keypuncher will merely transfer the information written in the Substance Coding Form to the corresponding columns on the computer card.

The Editor will also transcribe the substance name and number in the existing Master Materials Directory (the Master Alphabetical and Numerical Printouts of the Materials Directory).

D. FORMATS FOR THE SUBSTANCE CODING FORM

The following formats are to be used for the preparation of entries for the Materials Directory, including Synonyms and Cross-References. The Substance Coding Form, which has columns similar to a computer card, should be completed by the Editor accordingly.

Format 1. Substance Name, with or without formula (Series 1, 2, Classes 511, 513, 520, 521, 526, 535, 545, 551, 561 and Series 6).

| <u>Substance Entry</u> | <u>Card Column (cc) no.</u> | <u>Entry</u> |
|------------------------|-----------------------------|--|
| | cc 1 | TEPIAC Code C. |
| | 2-8 | Substance Number |
| | 18-19 | Card Number |
| | 20 | Operation Letter (<u>Add</u> , <u>Delete</u> or <u>Replace</u>) |
| | 21-80 | Substance Name (For Classes 511 and 513, break for next card must be at the plus sign (+), either before or after. All parts of any single component must be completely on one card.) |

TABLE 13. SUBSTANCE CODING FORM
(TEPIAC MATERIALS DIRECTORY ENTRIES AS KEYPUNCHED)

| | | | |
|----|-----------------|---|----|
| 1 | C 1 0 6 0 0 2 6 | 0 1 A C a l c i u m F l u o r i d e C a F (2) | 1 |
| 2 | | | 2 |
| 3 | | | 3 |
| 4 | C 5 1 3 0 0 0 1 | 0 1 A L e a d S u l f i d e (P b S) + L e a d T e l l u r i d e (P b T e) + | 4 |
| 5 | C 5 1 3 0 0 0 1 | 0 2 A T i n T e l l u r i d e (S n T e) | 5 |
| 6 | | | 6 |
| 7 | | | 7 |
| 8 | C 2 2 1 2 2 6 3 | 0 1 A 3 7 1 1 1 1 5 - T e t r a m e t h y l - 1 - h e x a d e c e n - 3 - o 1 | 8 |
| 9 | C 2 2 1 2 2 6 3 | 0 2 A C H (3) (C H C H (3) (C H (2)) (3)) (3) C C H (3) O H C H (2) | 9 |
| 10 | C 2 2 1 2 2 6 3 | 2 0 A 2 2 1 I i s o p h y t o l | 10 |
| 11 | | | 11 |
| 12 | | | 12 |
| 13 | C 1 0 2 0 3 3 1 | 0 1 A A l u m i n u m S i l i c a t e A l (2) S i O (5) | 13 |
| 14 | C 1 0 2 0 3 3 1 | 5 5 A 5 2 1 0 0 3 2 I a n d a l u s i t e | 14 |
| 15 | C 1 0 2 0 3 3 1 | 6 5 A 5 2 1 0 0 3 3 I c y a n i t e | 15 |
| 16 | C 1 0 2 0 3 3 1 | 8 0 A 1 0 2 0 0 2 1 M u l l i t e A l (2) S i O (5) | 16 |
| 17 | | | 17 |
| 18 | | | 18 |
| 19 | C 3 2 2 0 0 0 3 | 0 1 A F e + 0 - 1 0 0 C r | 19 |
| 20 | | | 20 |
| 21 | | | 21 |
| 22 | C 3 2 2 0 1 6 4 | 0 1 A 5 5 F e + 2 4 C r + 1 5 N i + 2 M n + . 2 C | 22 |
| 23 | C 3 2 2 0 1 6 4 | 0 2 A * S 3 0 9 0 0 | 23 |
| 24 | C 3 2 2 0 1 6 4 | 2 0 A 3 0 0 1 S 3 0 9 0 0 (2 4 C r) | 24 |
| 25 | C 3 2 2 0 1 6 4 | 2 1 A 3 0 0 1 A I S I 3 0 9 (2 4 C r) | 25 |
| 26 | | | 26 |
| 27 | | | 27 |
| 28 | C 4 0 3 0 7 4 5 | 1 2 A B r i t i s h B r y t a l | 28 |
| 29 | C 4 0 3 0 7 4 5 | 2 0 A 4 0 0 1 B r i t i s h B r y t a l | 29 |
| 30 | | | 30 |
| 31 | | | 31 |
| 32 | C 5 0 3 0 0 0 1 | 0 1 A S i O (2) A l (2) O (3) N a (2) O + K (2) O + O t h e r | 32 |
| 33 | C 5 0 3 0 0 0 1 | 0 2 A C e r a m i c | 33 |
| 34 | | | 34 |
| 35 | | | 35 |
| 36 | C 5 0 3 0 0 0 2 | 1 2 A C o r n i n g G l a s s 7 0 5 2 | 36 |
| 37 | | | 37 |
| 38 | | | 38 |
| 39 | C 5 0 3 0 0 0 3 | 1 2 A S c h o t t G l a s s B K 7 | 39 |
| 40 | C 5 0 3 0 0 0 3 | 2 0 A 5 0 3 1 B K 7 G l a s s | 40 |

| <u>*Synonym Entry</u> | | <u>Entry</u> |
|-----------------------------|-------|--|
| <u>Card Column (cc) no.</u> | | |
| cc | 1 | TEPIAC Code C |
| | 2-8 | Substance Number |
| | 18-19 | *Card Number |
| | 20 | Operation Letter (<u>A</u> dd, <u>D</u> elete or <u>R</u> eplace) |
| | 21-23 | Class Number |
| | 30 | Sequence Number |
| | 31-80 | Synonym |

| <u>**Cross-Reference Entry</u> | | <u>Entry</u> |
|--------------------------------|-------|--|
| <u>Card Column (cc) no.</u> | | |
| cc | 1 | TEPIAC Code C |
| | 2-8 | Substance Number |
| | 18-19 | **Card Number |
| | 20 | Operation Letter (<u>A</u> dd, <u>D</u> elete or <u>R</u> eplace) |
| | 21-27 | Substance Number |
| | 30 | Sequence Number |
| | 31-80 | Cross-Reference |

Format 2. Alloys (Series 3 and 4)

| <u>Substance Entry</u> | | <u>Entry</u> |
|-----------------------------|-------|---|
| <u>Card Column (cc) no.</u> | | |
| cc | 1 | TEPIAC Code C |
| | 2-8 | Substance Number |
| | 18-19 | Card Number (a) Card 01 for Composition and Card 02, 03, etc. for Substance Name, and (b) if no card 01, start with card 12 for name. |
| | 20 | Operation Letter (<u>A</u> dd, <u>D</u> elete or <u>R</u> eplace) |
| | 21-80 | Composition (01 Card). Maximum of 5 components with specific values and element symbols specified. The components will be separated by plus (+) signs. |
| | 21-80 | Substance Name (02, 03, etc., cards). To indicate that the composition on card 01 is a handbook value, start with asterisk and no space, then name (i. e., *AISI 309). Computer program will move * to proper place, move name left one space and start name with capital letter. |

* The card number for each Synonym entry is a unique two digit number between 20-50. In an alphabetical listing, the synonym will be followed by the word "see", and will refer to the substance name.

** The card number for a cross-reference entry is also a unique two digit number between 51-99. The card numbers determine the alphabetical arrangement of the cross-reference entries. Therefore, in assigning a card number for a cross-reference, one must allow for future cross-reference entries. In an alphabetical listing, the cross-references will follow the substance name with the words "see also".

Synonym EntryCard Column (cc) no.

cc 1
2-8
18-19
20
21-23
30
31-80

Entry

TEPIAC Code C
Substance Number
* Card Number
Operation Letter (Add, Delete or Replace)
Class Number
Sequence Number
Synonym

Cross-Reference EntryCard Column (cc) no.

cc 1
2-8
18-19
20
21-27
30
31-80

Entry

TEPIAC Code C
Substance Number
** Card Number
Operation Letter (Add, Delete or Replace)
Substance Number
Sequence Number
Cross-Reference

Format 3. Oxide Mixtures (Ceramics, Glasses and Slags - Class 503)Substance EntryCard Column (cc) no.

cc 1
2-8
18-19

20
21-80

21-80

Entry

TEPIAC Code C
Substance Number
Card Number (a) Card 01 for Composition and Card 02, 03, etc., for Substance Name, and (b) if no card 01, Substance Name will start with card 12.
Operation Letter (Add, Delete or Replace)
Composition (01 Card). Maximum of 5 components with formulas separated by plus (+) signs.
Substance Name (02, 03, etc. cards).

Synonym EntryCard Column (cc) no.

cc 1
2-8
18-19
20
21-23
30
31-80

Entry

TEPIAC Code C
Substance Number
* Card Number
Operation Letter (Add, Delete or Replace)
Class Number
Sequence Number
Synonym

* For explanation see previous page.
** For explanation see previous page.

Cross-Reference Entry
Card Column (cc) no.

cc 1
 2-8
 18-19
 20
 21-27
 30
 31-80

Entry

TEPLAC Code C
 Substance Number
 ** Card Number
 Operation Letter (Add, Delete or Replace)
 Substance Number
 Sequence Number
 Cross-Reference.

E. RULES FOR KEYPUNCHING

The Editor should consider the rules for keypunching when he (she) completes the Substance Coding Form. The rules are listed below followed by examples illustrating each rule.

1. A capital letter is preceded by a blank. When the letter is at the beginning of a line, the letter is automatically capitalized.
2. Subscript letter(s) and/or number(s) are written in parentheses. There are no blanks following the left parenthesis or preceding the right parenthesis.
3. A superscript is indicated by the word "superscript" followed by letter(s) and/or number(s).
4. A name enclosed in parentheses has a blank following the left parenthesis, and a blank preceding the right parenthesis.
5. Certain symbols and all Greek letters have to be written in words.

Examples:

| <u>Rule</u> | <u>Substance</u> | <u>Written/Keypunched as</u> |
|-------------|---|--|
| 1 | AAQ Graphite | A A Q Graphite |
| 2 | H ₂ SO ₄ | H(2) S O(4) |
| 3 | Tricyclo[2·2·1·0 ^{2,6}] heptane | Tricyclo(2·2·1·0 superscript 2, 6) heptane |
| 4 | Poly(methyl methacrylate) | Poly(methyl methacrylate) |
| 5 | % | Percent |
| | ' | Prime |
| | " | Double Prime |
| | α | Alpha |
| | β | Beta |
| | γ | Gamma |
| | Δ | Delta |

F. PROCESSING OF THE RECORDED INFORMATION

Every week the coders will submit the completed Technical Coding Forms, and the abstracts of the coded documents to the keypunchers. The keypunchers will keypunch the code lines from the Technical Coding Forms, and the bibliographic citation from the abstracts on computer cards.

** For explanation see page 37 .

Every two weeks the Editor will submit the completed Temporary Substance Number Form and the Substance Coding Form to the keypunchers. The keypunchers will keypunch the change of the Temporary Substance Number to the Actual Substance Number (from the Temporary Substance Number Form), and the substance number, name and any synonyms (from the Substance Coding Form) on computer cards.

The information on the computer cards will be stored on computer tapes. The Materials File will be updated in the first week of January, March, May, July, September, and November. At the same time new printouts will be generated: an alphabetical list for each coder, and a numerical list for the Editor.

The Temporary Substance Number Form and the Substance Coding Form will be returned to the Editor by the keypunchers. These will be filed separately in ring folders, and located in the Coding Room.

G. CHANGES IN SUBSTANCE ENTRIES

Occasionally there may be a duplication of substance entries. In such a case, the Editor merges one substance number with the second number. He (she) will use the Temporary Substance Number Form to make the merger. In the column with the heading "Temporary Substance Number", will be listed the number that is to be merged (i. e., this will be removed from the Materials Directory). In the column "Actual Substance Number" will be listed the substance number that will be retained for the Materials Directory.

Or a substance name may be changed at a later date. In this case, the Editor will use the Substance Coding Form. He (she) will record the substance number, the correct substance name, and the letter "R" (for Replace) in the Operations column 20.

If a substance is to be removed entirely from the Materials Directory, the Editor follows the procedure described above, but in the Operations column 20, the letter "D" (for Delete) is written.

The computer cards that will be keypunched will correct the information stored in the computer tapes. Any technical coding for the merged substance number will also be corrected.

PART III
THE WRITING STYLE FOR SUBSTANCE ENTRIES

There are many systems of chemical nomenclature used throughout the literature. TEPIAC generally conforms to the rules of the International Union of Pure and Applied Chemistry (IUPAC). However, these are not completely adaptable to the classification system; hence, TEPIAC has found it necessary to formulate some simple rules. Synonyms with the molecular formulas (to avoid duplication and confusion) will be recorded for materials which may be named in different ways.

The following rules, along with those of IUPAC, should be consulted in writing entries for the "Directory of Substances."

A. NONSTOICHIOMETRIC COMPOUNDS

The numerical subscripts (0.5 and above) of a nonstoichiometric compound will be rounded off to a whole number; atoms less than 0.5 will be indicated by letter subscripts n, x and y. (See page 46 for the priority order for the use of subscripts.) The compound will be listed under the nearest stoichiometric compound, with "nonstoichiometric" following the compound name. The molecular formula of the compound will be listed in parentheses after the word "nonstoichiometric". Examples are given below:

| <u>Nonstoichiometric Compound</u> | <u>Substance Entry (Name)</u> | <u>Substance Entry (Molecular Formula)</u> |
|-----------------------------------|---|--|
| a. $UO_{1.1}$ | Uranium Oxide, Nonstoichiometric | UO |
| b. $UO_{2.2}$ | Uranium Oxide, Nonstoichiometric | UO_2 |
| c. $Na_{0.92}NO_3$ | Sodium Nitrate, Nonstoichiometric | NaN_3 |
| d. $Fe_2Li_{0.2}Zn_{0.8}O_4$ | Iron Lithium Zinc Oxide, Nonstoichiometric | $Fe_2Li_nZnO_4$ |

B. NOMENCLATURE OF "INORGANIC" COMPOUNDS

- Binary compounds will be named by the element considered as metal preceding the nonmetal. For example:

| | | | |
|------|------------------|------|------------------|
| NaCl | Sodium Chloride | GaSe | Gallium Selenide |
| AlN | Aluminum Nitride | CdS | Cadmium Sulfide |

- Certain binary compounds have well-established names which will be retained. Examples are:

| | | | | | |
|-----------|----------|-----------|-----------|-----------|-----------|
| AsH_3 | Arsine | GeH_4 | Germane | PH_3 | Phosphine |
| As_2H_4 | Diarsine | Ge_2H_6 | Digermane | SbH_3 | Stibine |
| BH_3 | Borane | H_2O | Water | SiH_4 | Silane |
| B_2H_6 | Diborane | NH_3 | Ammonia | Si_2H_6 | Disilane |

3. Some compounds will be treated as binary compounds for naming purposes. This occurs primarily where negatively charged polyatomic ions (radicals) have special "-ide" ending names and are treated as if they were single atoms in naming their compounds. Some examples are:

| | | | |
|------|------------------|--------------------|-------------------|
| NaOH | Sodium Hydroxide | NH ₄ Cl | Ammonium Chloride |
| HCN | Hydrogen Cyanide | LiNH ₂ | Lithium Amide |

4. Valence is not indicated in naming simple compounds, as a general rule. For example, FeO and Fe₂O₃ are both named "Iron Oxide". There are a few exceptions to this rule:

| | | | |
|------------------|----------------------|-------------------------------|--------------------|
| CBr ₄ | Carbon Tetrabromide | Cl ₄ | Carbon Tetraiodide |
| CCl ₄ | Carbon Tetrachloride | H ₂ O ₂ | Hydrogen Peroxide |
| CF ₄ | Carbon Tetrafluoride | | |

5. Metallic compounds containing oxygen and another nonmetal have names ending in "-ate", "-ite". Examples are:

| | | | |
|-------------------|-------------------|------------------------------------|--------------------------|
| NaNO ₃ | Sodium Nitrate | KAg(NO ₂) ₂ | Potassium Silver Nitrite |
| MgSO ₄ | Magnesium Sulfate | | |

6. Multiple metallic compounds with only one nonmetallic component will be named with metals in alphabetical order followed by the nonmetal. The nonmetal will have an "-ide" ending. Examples:

| | | | |
|----------------------------------|-------------------|--------------------|--------------------------|
| Co ₂ FeO ₄ | Cobalt Iron Oxide | CaSbS ₂ | Antimony Calcium Sulfide |
|----------------------------------|-------------------|--------------------|--------------------------|

7. Multiple metallic-nonmetallic compounds will be named with the metals in alphabetical order followed by the nonmetals, also alphabetically arranged. The endings of the nonmetals will be "-ide" if no oxygen is present, and "-ate" or "-ite" if there is oxygen.

8. Compounds consisting of nonmetallic elements will be named in the order of their appearance in the following sequence:

B, Si, C, Sb, As, P, N, H, Te, Se, S, At, I, Br, Cl, O, F.

The last element of the compound will end in "-ide". Examples are:

| | |
|--------------------|---------------------------|
| SiClF ₃ | Silicon Chloride Fluoride |
| AsIS ₂ | Arsenic Sulfide Iodide |
| ClF ₃ | Chlorine Fluoride |

9. Water of hydration is ignored in substance entries since it is not consistently noted in the literature.

10. Ions -- No sign is used to designate the oxidation state of the central atom. The word "ion" is, however, indicated with the chemical name. For example, InI₄⁻¹ is entered as follows:

| | |
|------------------|------------------------|
| InI ₄ | Indium iodide (-1) ion |
|------------------|------------------------|

C. NOMENCLATURE OF "ORGANIC" COMPOUNDS

The naming of organic compounds is generally according to the rules of IUPAC (International Union of Pure and Applied Chemistry).

The following comments are relevant to the nomenclature of organic compounds:

1. All simple aliphatic hydrocarbons such as hexane, pentane, etc., are assumed to be normal, if not otherwise designated. Therefore, the letter "n-" does not precede the chemical name.
2. Prefixes
 - a. Di, tri, tetra, etc. precede simple radicals, such as dichloromethane.
 - b. Bis, tris, tetrakis, etc. precede only complex radicals; for example, 2,5-Bis-(2-ethylethoxy) hexane; Tris-(2-ethylbutyl) phosphate.
3. The Order of Radicals Within a Compound Name -- Single and compound radicals are arranged alphabetically. A radical prefix such as di, tri, etc. are considered in the alphabetization. For example:
2,4-Dimethyl-8-fluoro-7-phenylquinoline.
A compound radical is considered as a unit; for example, dimethylamino--. A prefix indicative of the number of compound radical units, such as bis(dimethylamino)--, is to be regarded in the alphabetization.
4. Stereoisomers
 - a. D, L, and DL represent molecular configuration and are noted with the compound name.
 - b. d, l, and dl represent optical rotation and are ignored in writing the compound name.
5. Ester Nomenclature -- The policy chosen by TEPIAC is to name the alcohol portion of an ester as a radical, not an alcohol; for example:
Propyl acetate, not Propanol acetate;
1,2,3-Trihydroxypropyl triacetate, not 1,2,3-Propanetriol triacetate.
Correct spacing within an ester name is important, for a misused space will result in an incorrect name. For example:
Methylphenyl acetate is $\text{CH}_3\text{COOC}_6\text{H}_4\text{CH}_3$
Methyl phenylacetate is $\text{C}_6\text{H}_5\text{CH}_2\text{COOCH}_3$

D. THE ABBREVIATED STYLE OF WRITING MOLECULAR FORMULAS

Molecular formulas are listed with substance entries for Series 1 and 2 and Class 511 (513). A formula is written in the shortest way possible.

1. Symmetrical portions of a formula are enclosed in parentheses and the number of units noted; for example:

Write $(\text{BeCl}_2)_2$ instead of $\text{BeCl}_2\text{BeCl}_2$;

$\text{Ba}[(\text{CH}_3)_2\text{CHC}_6\text{H}_4]_2$ instead of $(\text{CH}_3)_2\text{CHC}_6\text{H}_4\text{BaC}_6\text{H}_4\text{CH}(\text{CH}_3)_2$.

Straight chain hydrocarbons, compounds, or radicals with no substitution groups are exceptions (see rule 3 below).

2. Identical repeating units of straight chain hydrocarbons with substituted radicals or of branched hydrocarbons are written as a single unit in parentheses with the number of repetitive units indicated; for example:

Write $\text{CH}_3\text{CH}(\text{OH})\text{C}_3\text{H}_7$ instead of $\text{CH}_3\text{CH}(\text{OH})\text{CH}_2\text{CH}_2\text{CH}_3$;




$(\text{CH}_3)_3\text{CC}_2\text{H}_5$ instead of $\text{CH}_3(\text{CH}_3)\text{C}(\text{CH}_3)\text{CH}_2\text{CH}_3$.

3. Straight chain hydrocarbon compounds and radicals with no substitution groups are written in the following abbreviated form:

Write C_4H_{10} instead of $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$;

C_2H_6 instead of CH_3CH_3 .

4. Ring Compounds

a. Ring structures such as , , and  are expressed as C_6H_5 , C_6H_{11} , and $\text{C}_4\text{H}_4\text{N}$, respectively.

b. The ring structure appears first in the formula when it has one or more identical substitutional groups; for example: $\text{C}_6\text{H}_5\text{CH}_3$, $\text{C}_6\text{H}_{10}\text{Cl}_2$, etc.

c. The ring structure is used to separate two or more different substitutional groups; for example: $\text{CH}_3\text{C}_6\text{H}_4\text{OH}$, $\text{CH}_3\text{C}_6\text{H}_3(\text{Cl})\text{OH}$, etc.

d. Letter abbreviations for radicals are not used. For example, Me, Pr, Bu are not written in place of CH_3 , C_3H_7 , and C_4H_9 , etc.

5. Carboxylic acid and ester groups are written as COOH and COOR , not CO_2H and CO_2R .

6. Connective bonds and degree of saturation are not indicated; for example:

Write CHCH instead of $\text{CH}=\text{CH}$;

CH_3COOH instead of $\text{CH}_3\text{-COOH}$.

E. COMPLEXES

A complex has two or more different molecules attached to form a single coordination compound. A dot is used to separate the molecular formulas. The word "complex" is indicated with the name, and the components are listed alphabetically; molecular formula components are written as they appear in the paper.

If a formula is not noted in the paper, its components are listed in the same order as in the name.

| <u>Alphabetized Formula</u> | <u>Molecular Formula</u> | <u>Name</u> |
|---|---|--|
| CeCl ₃ H ₃ N | CeCl·nNH ₃ | (Ammonia-cerium chloride) complex |
| C ₂₁ H ₁₅ N ₁₁ O ₂₀ | (NO ₂) ₃ C ₆ H ₂ N (NO ₂)CH ₃ ·2CH ₂ C ₆ H ₂ (NO ₂) ₃ | [(N-Methyl-N,2,4,6-tetranitroaniline) - trinitrotoluene] complex |

F. SPECIAL ATTENTION TO POLYMER ENTRIES

1. Oligomers with a Known Number of Monomeric Units -- Definite molecular formulas can be written for oligomers with a known number of units. They are then entered in Series 1 or 2. For example, (BeO₃)₃ is Beryllium oxide, trimeric.
2. Polymers with an Unknown Number of Monomeric Units -- In Class 631 polymer components are listed by name only. Different molecular units within parentheses are arranged alphabetically. These polymers are identified as:
 - a. Copoly -- Polymer produced by the addition reaction of two different molecular units; for example: Copoly(ethylene-styrene).
 - b. Terpoly -- Polymer produced by the addition reaction of three different molecular units; for example: Terpoly(acrylonitrile-butadiene-styrene).
 - c. Poly -- Polymer produced by the condensation reaction of two or more molecular units; for example: Poly(ethylene glycol-terphthalic acid).

No indication is made of cross-linkage or termination of the polymer chain.

G. SPECIAL CASES OF SUBSTANCE NOMENCLATURE

1. Trade Names -- Trade names are important in all the Series. A substance designated by a trade name is listed under its generic name, if known, followed by the words "Commercial Designations". Certain well-known materials with specific commercial names will be assigned separate substance entries. These are the Graphites, certain Silicon Oxides (fused silica or fused quartz), and Polymers. In all cases, the trade names are recorded in the Synonyms Index.
2. Moisture Content -- TEPIAC does not distinguish between degrees of water content in a substance, e.g., moist, humid, or water saturated. A substance is considered to be dry or in its natural moisture state. Solutions supersaturated with solvent are entered in the general mixtures Class 511 (513).

H. THE USE OF SUBSCRIPTS

The subscripts n , x , and y are used to represent composition ranges in intermetallics and nonstoichiometric compounds. The priority order for the use of these subscripts is:

1. n $Mg_2Pb_nSn_{1-n}$
2. $n+x$ $Cu_{1-n-x}Ni_xZn_n$
3. $n+x+y$ $Eu_{3-n-x}Fe_{5-y}Ga_yTb_xY_nO_{12}$.

I. THE PUNCTUATION OF SUBSTANCE ENTRIES

The rules of punctuation must be observed precisely in both the coding and proof-reading of substance entries to ensure a well-ordered Directory of Substances.

1. Dashes

- a. Dashes are used to separate a "position" symbol from a compound name. These letters or numerals designate where a functional group is attached to the parent compound. They are listed below.

| | | | | | |
|-----|------|--------------|--------|---------|-----------|
| -m- | -D- | - α - | -tert- | -cis- | -1- |
| -N- | -L- | - β - | -sec- | -trans- | -2- |
| -o- | -DL- | - γ - | | | -3-, etc. |
| -p- | | | | | |

No space is left between the "position" symbol and the dash.

- b. A dash is used after *bis*, *tris*, and *tetrakis*, if these terms precede a "position" symbol; for example:

Bis-m-(methylbenzyl sebacate)
Bis-2-(ethylhexyl pimelate)

- c. A dash is not used to separate *bis*, *tris*, *tetrakis*, etc. from a radical name that has no position letter or number.

Bis(vinyloxy) methane

- d. Polymeric components are separated by a dash with a space left between the names and the dash.

Poly(ethylene glycol - terephthalic acid)

- e. A dash is used in front of a parenthesis when there is a position symbol within the parentheses; for example:

Bis-(2-methoxyethyl) phthalate
Poly-(1,1-Dichloroethylene)
Poly-(α -Chlorostyrene)

2. Parentheses

- a. Parentheses are used in compound names whenever their use clarifies the meaning; for example:

(Dimethyl phenyl) amine means $(CH_3)_2C_6H_5NH_2$, but
(Dimethyl) phenylamine means $(CH_3)_2NC_6H_5$.

- b. For polymers, parentheses are used when the polymer consists of a compound name, or contains more than one material. For example:

Poly(methyl methacrylate)
Poly(formaldehyde-melamine)

- c. Various descriptive terms such as "numbered series", "commercial designations", trade names in certain classes, etc. are enclosed in parentheses.
- d. With complex chemical formulas, more than one set of parentheses may be used.
3. Commas -- Commas are used mainly to separate lead words from descriptors.
4. Spacing -- Rules for spacing have been mentioned above in conjunction with the type of punctuation to which they are related.
5. The Singularity of Names -- All names are written in their singular form.

PART IV
PROCESSING OF TECHNICAL CODING

A. PROCEDURES IN TECHNICAL CODING

Each coder selects a group of papers to be coded. He (she) should check in the Index (Log Book) listing document numbers whether any paper has been coded already. For the uncoded documents the coder should collect their abstracts (in plastic folders) from the Input Control Documentalist. Before coding, the coder should check if a document and its abstract correspond in title, author(s), and the bibliographic citation. If they do not correspond, then the coder should consult the Input Control Documentalist. Any spelling corrections and the naming of a substance given only as a formula or abbreviation, may be done on the abstract itself.

The coder completes the Technical Coding Form consistent with the codes and classification criteria described in Part I, page 1. Every Wednesday the completed Technical Coding Forms are collected, assigned page numbers, and recorded in the Log Book as having been coded. Then these Technical Coding Forms, along with the abstracts of the coded documents, are submitted to the keypunchers for keypunching. The code lines from the Technical Coding Forms, and the bibliographic citation from the abstracts, will be keypunched on computer cards and the information stored on computer tapes. Periodically a numerical listing of all technical coding will be generated by the computer.

The Technical Coding Forms, returned by the keypunchers after processing, are filed in ring folders.

B. CHANGES IN TECHNICAL CODING

Occasionally a deletion may be needed for a code line keypunched and stored on a computer tape. (It may be for an incorrect code line, or for a duplicate code line arising from identical documents with different document numbers.)

The coder records exactly the code line to be deleted on the Technical Coding Form. In the Operations column 37, the letter "D" (for Delete) is written. The Technical Coding Form is then given to the keypunchers for processing. The computer card with the letter "D" in column 37 will delete the code line stored on the computer tape.

The corrected or an additional code line is entered in the Technical Coding Form, keypunched by the keypunchers, and stored on computer tapes.

PART V

THE EXCLUSION OF UNCODABLE DOCUMENTS FROM THE SYSTEM

Sometimes the coder will receive a document which does not contain suitable coding material according to the criteria in this manual. In such a case, the coder confers with the person who originally approved the paper for TEPIAC's classification system. If it is decided that the paper is an "out", the coder initials the document and abstract. The paper is recorded in the Index (Log Book) listing document numbers as being an "out". The document is then given to the Input Control documentalist to be flagged as an "out" in the Duplicate Search File.

APPENDIX I

A REVIEW OF THE THERMOPHYSICAL PROPERTIES

TEPIAC has chosen to investigate the literature for 14 thermophysical properties. An outline of the currently coded property symbols, equations, and related terms is presented in Table 14 at the beginning of this review. A brief discussion of each property follows.

Throughout this property review, related and unrelated terms are stated as "guide words" to aid the coder in property identification. Property units must always be carefully checked. If there is some doubt as to the advisability of accepting a term as a codable property, the matter should be discussed with a property specialist for a definite decision.

TABLE 14. THE THERMOPHYSICAL PROPERTIES

| Property | A. Thermal Conductivity | B. Accommodation Coefficient | C. Thermal Contact Resistance | D. Thermal Diffusivity | E. Specific Heat at Constant Pressure | F. Viscosity |
|---------------------------------|--|--|--|---|--|--|
| Defining Equation | $k = \frac{q}{dT/dx}$ | $\alpha = \frac{T_r - T_i}{T_w - T_i}$ | $h_c = \frac{Q}{A\Delta T}$ | $\alpha = \frac{k}{\rho C_p}$ | $C_p = \frac{\delta Q}{dT}$ | $\mu = \frac{F}{A} \frac{dZ}{dV}$ |
| Units | cal sec ⁻¹ cm ⁻¹ °C ⁻¹ joule sec ⁻¹ cm ⁻¹ °F ⁻¹ BTU hr ⁻¹ ft ⁻¹ °F ⁻¹ Watt cm ⁻¹ °K ⁻¹ | Dimensionless | cal cm ² °C ⁻¹ sec ⁻¹ BTU ft ⁻¹ °F ⁻¹ hr ⁻¹ Watt cm ⁻² °C ⁻¹ | cm ² sec ⁻¹ ft ² sec ⁻¹ | cal gm ⁻¹ °C ⁻¹ joule gm ⁻¹ °K ⁻¹ BTU lb ⁻¹ °F ⁻¹ cc-atm/gm | dyne sec cm ⁻² = poise centipoise poundal sec ft ⁻² |
| Related Symbols and Terms | Change in t. c. * Δk Collision integrals (theory) Effective t. c. Frozen t. c. Heat conduction Heat conductivity Lattice t. c. Lorenz function or number (theory) Phonon t. c. Reduced t. c. (or resistivity) t. c. ratio k_g/k_n Thermal magneto- resistance† Thermal resistiv- ity (reciprocal of t. c.) Translational t. c. | Momentum accom- modation coef- ficient Temperature dis- continuity effect (theory) Temperature jump effect (theory) | Electrical contact resistance (theory) Heat conductance (valid only if measurement is of a <u>contact</u>) Kapitza conduc- tance (resis- tance) Thermal contact conductance Thermal resis- tance (recipro- cal of heat con- ductance, should be of a <u>contact</u>) Thermal boundary resistance | Thermometric conductivity Temperature con- ductivity (term used in foreign translations) | Apparent s. h. ** Atomic heat Change in s. h. ΔC_p C_n, C_p Cv of solids at <15°K Debye tempera- ture vs. temper- ature Electronic s. h. Enthalpy vs. tem- perature Excess s. h. Heat (thermal) capacity Heat content with Cp formula Isobaric Cp Lattice s. h. Magnetic s. h. Mean s. h. Molar s. h. Nuclear s. h. Reduced s. h. Saturated s. h. Schottky s. h. Vibrational heat capacity | Absolute v. *** Bulk v. Collision integrals (theory-only if viscosity men- tioned) Dynamic v. Fluidity (Φ) Kinematic v. Mean v. Melt v. Nsp Relative v. (if sol- vent value known) Shear v. Superfluidity Viscosity coeffi- cient Volume v. |

* t. c. - thermal conductivity

** s. h. - specific heat

*** v. - viscosity

† refer to a property specialist

TABLE 14. (continued)

| Property | A. Thermal Conductivity | B. Accommodation Coefficient | C. Thermal Contact Resistance | D. Thermal Diffusivity | E. Specific Heat at Constant Pressure | F. Viscosity |
|--------------------|--|--|---|---|---|--|
| Unrelated Terms | Electrical conduc- tivity Heat (thermal) conductance (check units) Heat transfer coefficient Temperature con- ductivity (prop- erty D) Thermal resist- ance (property C) | | Electrical conduc- tance Heat (thermal) conductivity (check units) Heat transfer coefficient Temperature con- ductivity (prop- erty D) Thermal resist- ivity | Diffusion coeffic- ient Diffusion thermo- effect Thermal diffusion coefficient Thermal diffusion factor (α) | Cp-Cv Cp/Cv Cv of gases and liquids Entropy Gibbs free energy values Grüneisen con- stant Heat content w/o Cp formula Heat (enthalpy) of formation or fusion Specific heat dur- ing a reaction | Apparent v. Creep Eddy v. of mo- mentum Film coefficient Intrinsic v. Magnetic v. Mooney v. Second v. Shear coefficient Solid v. Surface v. Turbulent v. Viscoelasticity Liquid phase of organic com- pounds Oils and lubricants Oxide mixtures (ceramics, glasses, and slags) Polymers Suspensions (slurries) |
| Exclusions | Unsteady state | | | | | |
| Remarks | | Enter in Systems Class 535 as "Gas on Solid" | Enter in Systems Class 535 | | | |

TABLE 14. (continued)

| Property | G. Emittance | H. Reflectance | I. Absorbance | J. Transmittance | K. Absorbance to Emittance Ratio |
|---------------------------|---|--|--|--|--|
| Defining Equation | $\epsilon = \alpha + \rho$ | $\rho = \frac{I_r}{I_o}$ | $\alpha = \frac{I_a}{I_o}$ | $\tau = \frac{I_t}{I_o}$ | $\alpha/\epsilon = \text{Ratio of absorbance to emittance}$ |
| Units | Dimensionless May be expressed in percentage or fractional terms | Dimensionless May be expressed in percentage or fractional terms | Dimensionless May be expressed in percentage or fractional terms | Dimensionless May be expressed in percentage or fractional terms | Dimensionless |
| Related Symbols and Terms | Degree of blackness (Russian papers) Emissive power Emissivity | Albedo Electrorreflectance Magnetorelectance Optical reflectivity Plasma edge reflectance Radiance factor Reflectance factor Reflection amplitude Reflection coefficient Reflection of radiation Reflection spectra Reflectivity Thermoreflectance | Absorbance Absorptivity Absorption spectra (if property clearly defined) Infrared spectra (if property clearly defined) | Absorption spectra (if property clearly defined) Attenuated total reflectance (ATR) Infrared spectra Opacity Optical Density Optical Transmittance Optical Transparency Transmission Transmission of radiation Transmissivity | Alpha over epsilon Normal solar absorbance/hemispherical total emittance Solar radiation coefficient |
| Unrelated Terms | Spectra (arbitrary units) or band studies Emission Emission coefficient Emittance (tons) | Spectra (arbitrary units) or band studies Optical property | Spectra (arbitrary units) or band studies Absorbance index Absorbancy Absorption coefficient Index of absorption Molar absorbance index Optical Absorbancy | Spectra (arbitrary units) or band studies Transmittancy Transmission (electrons) | |
| Exclusions | | | | | Liquids, gases, organic substances (except polymers), inorganic complexes, and adsorbed materials. |

TABLE 14. (continued)

| Property | L. Prandtl Number | N. Thermal Linear Expansion Coefficient | O. Thermal Volumetric Expansion Coefficient |
|---------------------------|---|---|---|
| Defining Equation | $Pr = \frac{C_p \mu}{k}$ | $\alpha = \frac{L_2 - L_1}{L_0(\Delta T)}$ | $\beta = \frac{V_2 - V_1}{V_0(\Delta T)}$ |
| Units | Dimensionless | $\text{cm } ^\circ\text{C}^{-1}$ $\text{ft } ^\circ\text{F}^{-1}$ | $\text{cm}^3 \text{ } ^\circ\text{C}^{-1}$ $\text{ft}^3 \text{ } ^\circ\text{F}^{-1}$ |
| Related Symbols and Terms | Pr | Diametral expansion Dilatation Elongation percent (if zero stress) Isobaric linear thermal expansion $\Delta L/L$ vs. temperature graph Lattice constant vs. temperature Lattice parameter linear expansion Length vs. temperature graph Percent expansion (linear) Thermal expansion (linear) Thermal linear contraction | Cubic expansion coefficient Cubic lattice constant vs. temperature graph Density vs. temperature Change in density ($\Delta\rho/\rho$) vs. temperature (even one value) Isobaric volumetric expansion Percent expansion (volumetric) Thermal expansion (volumetric) $\Delta V/V$ vs. temperature graph Volume vs. temperature graph Grüneisen constant Liquid or gas volume expansion |
| Unrelated Terms | Grashof number Nusselt number Reynolds number | | |
| Exclusions | | | Liquids and gases |

THERMAL CONDUCTIVITY (A)

Heat conduction is the phenomenon of thermal energy transmission from one point to another in a stationary medium that is not at uniform temperature. This process of heat conduction takes place within liquids, gases, and solids.

Experimental studies of heat conduction have demonstrated that the amount of heat conducted in a medium is directly proportional to the cross-sectional area of the medium normal to heat flow, the temperature gradient (which is the spatial rate of change of temperature) of the medium in the direction of heat flow, and the time during which the temperature gradient is maintained:

$$Q \propto A \frac{dT}{dx} \tau \quad \text{where} \quad \begin{array}{l} Q = \text{amount of heat} \\ A = \text{cross-sectional area} \\ \frac{dT}{dx} = \text{temperature gradient} \\ \tau = \text{time elapsed} \end{array}$$

By introducing the proportionality factor k , the coefficient of thermal conductivity, one can write

$$Q = k A \frac{dT}{dx} \tau, \quad (\text{I-1})$$

valid for unidirectional steady-state conduction. It follows that

$$k = \frac{Q}{A \frac{dT}{dx} \tau} = \frac{q}{\frac{dT}{dx}}, \quad (\text{I-2})$$

where q is the heat conducted per unit time across unit cross-sectional area. The thermal conductivity k is thus the quantity of heat conducted per unit time through unit area normal to the direction of heat flow per unit temperature gradient.

$$\begin{array}{l} \text{In metric units,} \quad k = \text{cal sec}^{-1} \text{ cm}^{-1} \text{ } ^\circ\text{C}^{-1} \\ \quad \quad \quad \quad \quad k = \text{joule sec}^{-1} \text{ cm}^{-1} \text{ } ^\circ\text{K}^{-1} \end{array}$$

$$\text{In British units,} \quad k = \text{BTU hr}^{-1} \text{ ft}^{-1} \text{ } ^\circ\text{F}^{-1}$$

$$\text{In electrical units,} \quad k = \text{Watt cm}^{-1} \text{ } ^\circ\text{K}^{-1}$$

Thermal conductivity is dependent upon the type of material, the temperature and pressure, as well as sample purity (or composition), density (or porosity), crystal imperfection, crystal axis orientation, thermal history, microstructure, etc.

In an electrical conductor such as a pure metal, heat is conducted primarily through the motion of free electrons, though there is also a contribution due to lattice vibrations which is generally small. The portion of thermal conductivity due to the contribution

of free electrons is called electronic thermal conductivity while that due to the contribution of lattice vibrations is called lattice thermal conductivity or phonon thermal conductivity. The quanta of vibrational energy are called phonons in analogy to photons, the quanta of radiant energy.

The thermal conductivity of metals increases with the number of free electrons and with their mean free path, which is the average distance an electron travels before it is diverted by collisions with impurities or lattice imperfections, or by interactions with the thermal vibrations of the lattice.

In dielectric solids, heat is conducted by lattice vibrations since their electrons are not free to move through the lattice structure. Thermal conductivity here is determined by the number and mean free path of phonons. At very high temperatures, non-metallic solids may also conduct heat in other ways, as by electrons freed by thermal excitation, and by direct radiant heat transport by photons.

Solid materials intermediate between electrical conductors and insulators have thermal conduction due to both free electrons and lattice vibrations in varying degrees, depending upon whether they are closer to being electrical conductors or insulators. Heat energy is conducted in liquids and gases by molecular collisions.

The Lorenz function (or Lorenz number) is closely related to the thermal conductivity and is included with this property code, as theory only. Wiedemann and Franz found that at room temperature the ratio of thermal conductivity to electrical conductivity, k/σ , of metals is approximately a constant. This relation is the Wiedemann-Franz law:

$$\frac{k}{\sigma} \approx \text{constant} \quad (1-3)$$

Lorenz found that in addition to the Wiedemann-Franz ratio's being approximately a constant at a given temperature, it was also directly proportional to the absolute temperature. This results in the Wiedemann-Franz-Lorenz law:

$$\frac{k}{\sigma} = LT \quad (1-4)$$

where the Lorenz function L is

$$L = \frac{k}{\sigma T} \quad (1-5)$$

The Lorenz function is usually a weak function of temperature and varies slightly for different kinds of metals.

The following related terms may be coded as thermal conductivity (property A) if they are clearly defined.

Change in thermal conductivity Δk
 Collision integrals (theory)
 Effective thermal conductivity
 Frozen thermal conductivity
 Heat conduction
 Heat conductivity
 Lattice thermal conductivity
 Lorenz function or number (theory)
 Phonon thermal conductivity
 Reduced thermal conductivity (or resistivity)
 Thermal magnetoresistance (in $\text{watt cm}^{-1} \text{ } ^\circ\text{K}$) - When this term is encountered, it should be brought to the attention of the consultant to determine if it is codable.
 Thermal resistivity (reciprocal of thermal conductivity)
 Translational thermal conductivity
 Thermal conductivity ratio k_s/k_n $\left\{ \begin{array}{l} s = \text{superconducting state} \\ n = \text{normal state} \end{array} \right\}$

The following terms should not be coded as thermal conductivity:

Electrical conductivity (in ohm cm^{-1})
 Heat (or thermal) conductance (in $\text{watt cm}^{-2} \text{ } ^\circ\text{K}^{-1}$) - This term may be coded as thermal contact resistance only if it is used in context with contacts. Therefore, it is pertinent that units be checked before any coding decision is made.
 Heat transfer coefficient
 Temperature conductivity - see thermal diffusivity (property D)
 Thermal resistance (in $\text{watt}^{-1} \text{ cm}^2 \text{ } ^\circ\text{K}$)

For informative review articles see:

1. "The conduction of heat in solids," R. L. Sproull, Sci. Amer. 207, 92-104 (1962), TPRC 48285.
2. "The thermal properties of materials," J. Ziman, Sci. Amer. 217, 180-188 (1967), TPRC 46495.

ACCOMMODATION COEFFICIENT (B)

The accommodation coefficient represents the fractional extent to which gas molecules being reflected from a solid surface are able to equilibrate their temperature with that of the solid.

Thermal energy in gases is transferred by random molecular collisions. A gas molecule will traverse different distances between two successive collisions. The average distance that a molecule travels between successive collisions is called the "mean free path." As the pressure within the container is reduced, the density of the molecules decreases and the mean free path increases. When the mean free path approaches the size of the container, the normal mechanism of heat transfer is altered.

Consider a heated axial wire in a cylinder filled with a gas at a pressure such that the mean free path is larger than the diameter of the wire, but much less than the distance of the wire from the cold wall of the container. The probability that molecules that strike the wire will have come directly from a collision with the cold wall will be small. Their most recent collisions will have been with gas molecules a few mean-free-path lengths from the wire, and their average energy will be determined by the energies of those molecules. The molecules incident on the wire will thus have energies corresponding to a temperature T_i that is somewhat less than the temperature T_w of the wire itself. During their collision with the wire the reflected molecules will have gained energy and will have been brought to an effective temperature T_r , higher than T_i , but usually still less than T_w . One may say that there is an incomplete accommodation of the temperature of the reflected molecules to that of the wire. The accommodation coefficient α , defined as

$$\alpha = \frac{T_r - T_i}{T_w - T_i}, \quad (1-6)$$

is a measure of the degree to which accommodation takes place. For complete accommodation $T_r = T_w$ and $\alpha = 1$. In practical cases α is less than 1. This affects the conduction of heat away from the wire by the gas, modifying the temperature distribution in the gas near the wire, and actually introducing a discontinuity between the temperature in the gas as the wire is approached and the temperature of the wire itself. This is known as the "temperature jump effect" or "temperature discontinuity effect."

The value of α is sensitive to small changes in the nature of the solid surface, and therefore is often used to obtain valuable information about changes in the state of the surface.

Substance entries for this property are indexed in the systems Class 535 as "Gas on solid"; for example, Helium on tungsten.

The following terms may be coded for thermal contact resistance, if they are clearly defined:

Momentum accommodation coefficient
Temperature discontinuity effect (theory)
Temperature jump effect (theory)

THERMAL CONTACT RESISTANCE (C)

In most heat transfer experiments, heat is conducted through layered walls with different materials in contact. Precise heat transfer calculations require that the heat resistance offered at the interface of contact surfaces be considered.

The thermal resistance of a contact pair is mainly a surface effect, with magnitude determined by the structure of the surfaces, as well as the thermal and mechanical properties of the materials involved. An ideal contact in a vacuum having two perfectly planed surfaces in intimate contact would exhibit no extra resistance at the interface. The heat flow through an ideal contact would have a continuous temperature distribution (see Fig. I-1).

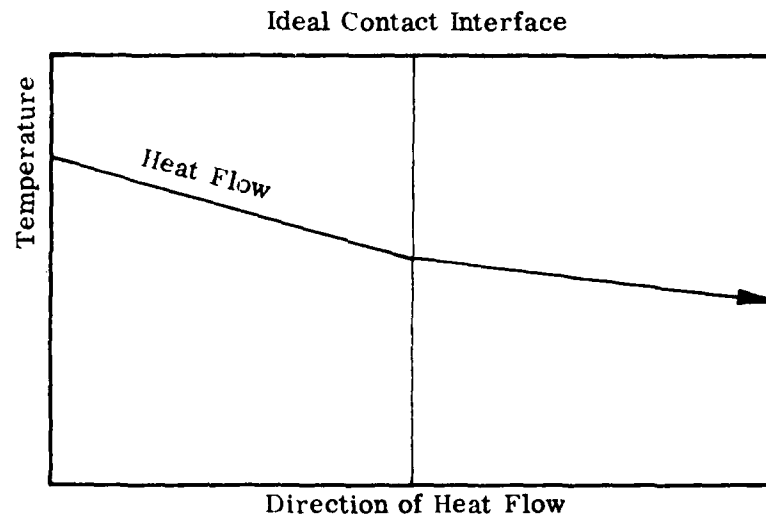


Fig. I-1

Real contact surfaces are never perfectly planed. Even highly polished surfaces have minute irregularities which appear as a succession of jagged hills. When two metallic surfaces are pressed together, intimate contact is made only at the points of these hills. The thermal conductivity of the contact materials is generally greater than the thermal conductivity of the material or fluid (liquid or gas) filling the interstices. Since heat flow tends to follow the path of least thermal resistance, most of the heat will be channeled through the contact points, and only a small amount of heat will cross the more resistant gaps. (See Fig. I-2.)

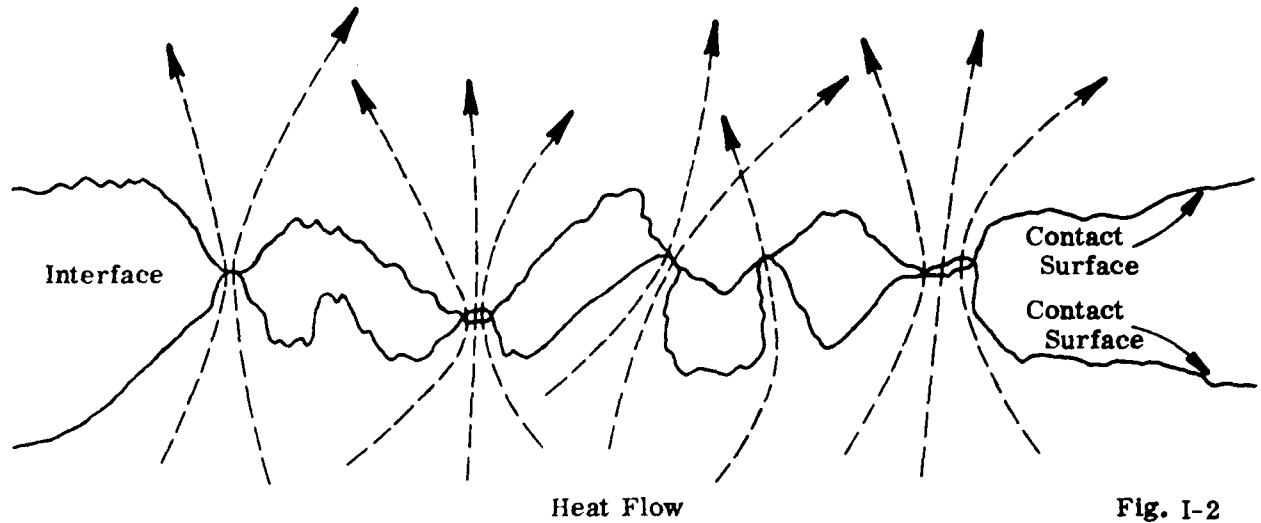


Fig. I-2

Therefore, the temperature drops sharply across the interstices. This rapid change in temperature can be idealized as a temperature discontinuity, as illustrated in Fig. I-3.

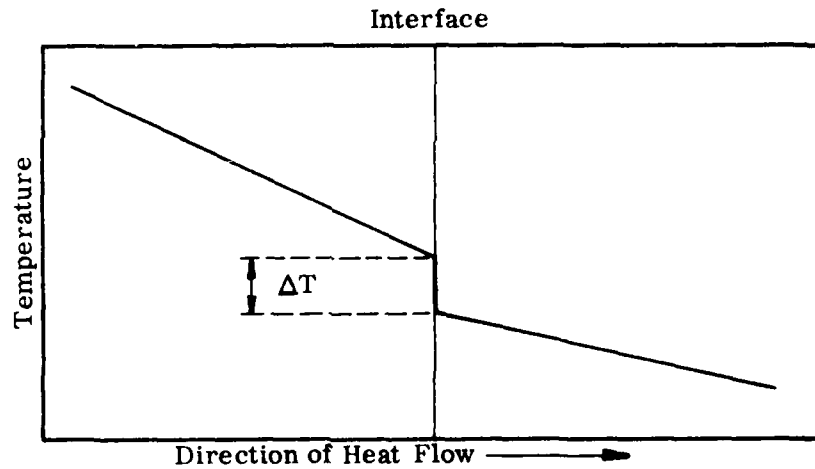


Fig. I-3

The effect of the sharp drop in temperature between the contact surfaces can be expressed in terms of a thermal contact resistance, or its reciprocal, the thermal contact conductance. The thermal conductance of the contact is defined as the ratio

$$h_c = \frac{Q}{A \Delta T}, \quad (\text{I-7})$$

where Q/A is the heat Q flowing per unit time across the projection area A of the contact (the apparent area, not the microscopic actual area of intimate contact) and ΔT is the additional temperature drop due to the contact surface. ΔT can in some cases be obtained

experimentally by extrapolating the temperatures in the bulk materials, observed outside the region of flow disturbance, down to the contact surface.

In metric units, $h = \text{cal cm}^{-2} \text{ } ^\circ\text{C}^{-1} \text{ sec}^{-1}$

In British units, $h = \text{Btu ft}^{-2} \text{ } ^\circ\text{F}^{-1} \text{ hr}^{-1}$

In electrical units, $h = \text{watt cm}^{-2} \text{ } ^\circ\text{C}^{-1}$

Contacts are considered by their physical nature as "systems" and are entered into Class 535. The fluid or coating, if any, at the interface of two surfaces is noted as "with filler" on the strip along with the contact substances. An example of such an entry is Copper-Magnesium oxide, with filler. Only the property code letter C will identify the materials as contacts.

Terms that are related to and coded as thermal contact resistance if clearly defined are:

Electrical contact resistance (coded for theory)

Heat conductance - The units for this term and thermal contact conductance are identical. It is valid for coding as property C only if the property measurement is of a contact. Sometimes this term is misused in foreign translations to mean thermal conductivity (property A); therefore, property units must always be checked.

Kapitza conductance (resistance)

Thermal contact conductance

Thermal resistance - The comments above for its reciprocal, heat conductance, are true also for this term.

Terms that are not coded as thermal contact resistance are:

Electrical conductance

Heat (or thermal) conductivity

Heat transfer coefficient - This term has the same units as thermal contact conductance, but since it is a measure of heat transfer from a solid to a fluid, or vice versa, it is not considered equivalent to Property C.

Temperature conductivity

Thermal resistivity

THERMAL DIFFUSIVITY (D)

Thermal diffusivity can be defined as the rise in temperature produced in a unit volume of substance by the amount of heat flowing per second through a unit area under a unit temperature gradient. Since the amount of heat flowing per unit time through a unit area under a unit temperature gradient is just equal to the thermal conductivity k of the material (Eq. I-1), and the thermal capacity of a unit volume of the material (at constant pressure) is ρC_p , where ρ is the mass per unit volume and C_p is the specific heat, it follows from Eq. (I-9) that the thermal diffusivity α is given by

$$\alpha = \frac{k}{\rho C_p} \quad (\text{I-8})$$

In metric units, $\alpha = \text{cm}^2 \text{sec}^{-1}$

In British units, $\alpha = \text{ft}^2 \text{sec}^{-1}$

Thermal diffusivity should not be confused with mass diffusivity which has the same units. Mass diffusivity is concerned with bulk transport due to a concentration gradient, while thermal diffusivity is concerned with heat transport due to a temperature gradient.

The following terms are related to thermal diffusivity and accepted for coding, if clearly defined:

Thermometric conductivity
Temperature conductivity - This term is often used in foreign translations.

The following terms are not coded as thermal diffusivity:

Diffusion coefficient
Diffusion thermoeffect
Thermal diffusion coefficient
Thermal diffusion factor (α)

SPECIFIC HEAT AT CONSTANT PRESSURE (E)

The thermal capacity of any mass m of a substance is the quantity of heat required to raise its temperature by one degree. More precisely, its mean thermal capacity in the temperature range T_1 to T_2 is defined by

$$\bar{c} = \frac{Q'}{T_2 - T_1}, \quad (\text{I-9})$$

where Q' is the heat that must be added (usually under some specified conditions of pressure or volume) to raise the temperature from T_1 to T_2 .

A corresponding but simpler quantity is the specific heat, which is the average thermal capacity of unit mass of the substance in a very small temperature range ΔT about temperature T :

$$C = \frac{\Delta Q'/m}{\Delta T} = \frac{\Delta Q}{\Delta T}, \quad (\text{I-10})$$

where ΔQ is the heat absorbed per unit mass. This ratio depends on the temperature, and on the conditions under which the heating is carried out. For instance, the heat that must be added when the substance is heated under constant pressure, ΔQ_p , is usually different from the heat ΔQ_v that must be added when it is heated at constant volume. One must therefore distinguish the specific heat at constant pressure, which in the notation of infinitesimals may be written

$$C_p = \frac{\delta Q_p}{dT} \equiv \left(\frac{\delta Q}{\delta T} \right)_p \equiv \left(\frac{dQ}{dT} \right)_p, \quad (\text{I-11})$$

from the specific heat at constant volume

$$C_v = \frac{\delta Q_v}{dT} \equiv \left(\frac{\delta Q}{\delta T} \right)_v \equiv \left(\frac{dQ}{dT} \right)_v. \quad (\text{I-12})$$

One writes δQ or dQ instead of simply dQ to keep in evidence the fact that one is not dealing with an increment dQ of some function Q that depends only on the state of the system, but with an added heat δQ that depends on the precise way in which the state of the system is changed.

There is no uniquely defined "total heat content Q " of a unit mass, of which C_v and C_p may be regarded as ordinary partial derivatives with respect to T . There is, however, a state function, the internal energy (often denoted by E), of which C_v is an ordinary partial derivative,

$$C_V = \left(\frac{\partial E}{\partial T} \right)_V, \quad (I-13)$$

and another state function, the enthalpy H , of which C_p is an ordinary partial derivative,

$$C_p = \left(\frac{\partial H}{\partial T} \right)_p. \quad (I-14)$$

For matter subject only to simple hydrostatic pressure p ,

$$H = E + pV. \quad (I-15)$$

The quantities E and H are often tabulated, and one can derive C_p and C_V from such tables. It is common to tabulate H in terms of its change from a reference temperature, usually 298.15°K , giving $H_T - H_{298.15}$ as a function of T for various fixed pressures. Then one can easily derive

$$C_p = \left[\frac{d(H_T - H_{298.15})}{dT} \right]_p. \quad (I-16)$$

The units of specific heat (whether at constant volume or constant pressure) are as follows:

In metric units, $\text{cal gm}^{-1} \text{ } ^\circ\text{C}^{-1}$, or $\text{joule gm}^{-1} \text{ } ^\circ\text{C}^{-1}$

In British units, $\text{BTU lb}^{-1} \text{ } ^\circ\text{F}^{-1}$.

The units of internal energy and of enthalpy are:

In metric units, cal gm^{-1} , or joule gm^{-1}

In British units, BTU lb^{-1} .

A common practical unit is $\text{cc} - \text{atm/gm}$.

DIFFERENCE BETWEEN C_p AND C_V

From consideration of thermodynamics:

$$C_p - C_V = -T \left(\frac{\partial V}{\partial T} \right)_p^2 / \left(\frac{\partial V}{\partial p} \right)_T \quad (I-17)$$

The coefficient of volumetric expansion is

$$\beta = \left(\frac{\partial V}{\partial p} \right)_T / V \quad \text{and} \quad (I-18)$$

the isothermal compressibility is

$$K_T = - \left(\frac{\partial V}{\partial p} \right)_T / V, \quad (I-19)$$

so Eq. (I-17) becomes

$$C_p - C_V = \frac{TV\beta^2}{\kappa_p}, \quad (\text{I-20})$$

Equation (I-20) may also be written as

$$C_p - C_V = \left(\frac{V\beta^2}{\kappa_p C_p^2} \right) C_p^2 T = AC_p^2 T \quad (\text{I-21})$$

where $A = \frac{V\beta^2}{\kappa_p C_p^2}$ is called the Grüneisen "constant", a parameter which is nearly constant over a wide range of temperature.

The specific heat at constant volume is approximately equal to the specific heat at constant pressure at $< 15^\circ\text{K}$. Above this temperature, C_V may no longer be assumed to be equal to C_p .

THE ATOMIC THEORY OF SPECIFIC HEAT

The heat absorbed by a material appears, on an atomic scale, as kinetic energy of its constituent molecules, atoms, and electrons and as potential energy of their interactions with each other. The first reasonably successful theories of the specific heats of solids treated the atoms of solid elements as harmonic oscillators, and led to the conclusion that their specific heats would all be 6 calories per gram atom per degree Centigrade. This result (the Law of Dulong and Petit) is approximately valid at high temperatures, but fails at low temperatures, where the specific heat goes to zero. Einstein's explanation of this in terms of the quantum theory was a big step in the demonstration of the need for quantum theory in the treatment of atomic systems. The full modern theory of specific heat is quite complex, since this property is affected by many details of the atomic structure and of the interactions of the atomic particles, in ways that vary from one class of materials to the next. Analytic approximations are sometimes very useful. For instance, the specific heat of a solid at constant volume and at low (but not too low) temperatures can sometimes be usefully represented by

$$C_V = \gamma T + \beta T^3 + \alpha T^{-2}, \quad (\text{I-22})$$

where α , β , and γ are constants, and the successive terms on the right are connected with the behavior of the electrons, of the vibrating atomic lattice, and of the atomic nuclei. There does not, however, exist any such expression with general validity.

The following terms and symbols are related to specific heat at constant pressure and coded as property E, if clearly defined:

| | |
|--------------------------------------|--|
| Apparent specific heat | Heat content - If C_p can be calculated from formula |
| Atomic heat | Lattice specific heat |
| Change in specific heat ΔC_p | Magnetic specific heat |
| C_n , C_p | Mean specific heat |
| C_v of solids at $< 15^\circ K$ | Molar specific heat |
| Debye temperature vs temperature | Nuclear specific heat |
| Electronic specific heat | Reduced specific heat |
| Enthalpy vs temperature | Saturated specific heat |
| Excess specific heat | Schottky specific heat |
| Heat (or thermal) capacity | Vibrational heat capacity |

The following terms and symbols are not coded as C_p :

$C_p - C_v$
 C_p / C_v
 C_v of gases and liquids
 Entropy
 Grüneisen constant
 Heat content values with no formula for C_p calculation

If the specific heat of a gas or liquid is measured while it is adsorbed on a solid substrate the substance is entered in the appropriate class for the gas or liquid, with an accompanying notation about the substrate. For example: Helium adsorbed on Titanium oxide (TiO_2); Neon, adsorbed on xenon, adsorbed on graphite. (For specific heat only, an adsorbed liquid or gas is not considered a "system"; hence, entries are made according to the adsorbate.)

For an informative review see:

"Einstein, Specific Heats, and the Early Quantum Theory," M. T. Klein, Science, 148(3667), 173-80 (1965), TPRC No. 36152.

VISCOSITY (F)

During the laminar flow of a liquid, there occurs a relative shearing motion between its molecular layers that results in a certain amount of resistance to the flow. This resistance to flow, termed viscosity, varies greatly among liquids.

Consider a liquid between two parallel plates subject to parallel relative displacement with velocity V_{\max} (see Fig. I-4). The velocity of flow relative to the bottom plate changes from 0 in the layer adhering to the bottom plate to V_{\max} in the layer adhering to the top plate. In ideal laminar flow the velocity V in a layer at distance Z from the bottom plate will be proportional to Z ; dV/dZ will be constant. The opposed (shearing) forces F on the plates required to maintain this uniform distribution of relative velocities is called the viscous force. It is proportional to the area A of the plates, and to dV/dZ . By introducing a proportionality constant μ , called the coefficient of viscosity, one can write

$$F = \mu A \frac{dV}{dZ}, \quad (\text{I-23})$$

$$\mu = \frac{F}{A} \frac{dZ}{dV}. \quad (\text{I-24})$$

Equation (I-23), with μ a constant, is Newton's law for viscous streamline (as opposed to turbulent) flow.

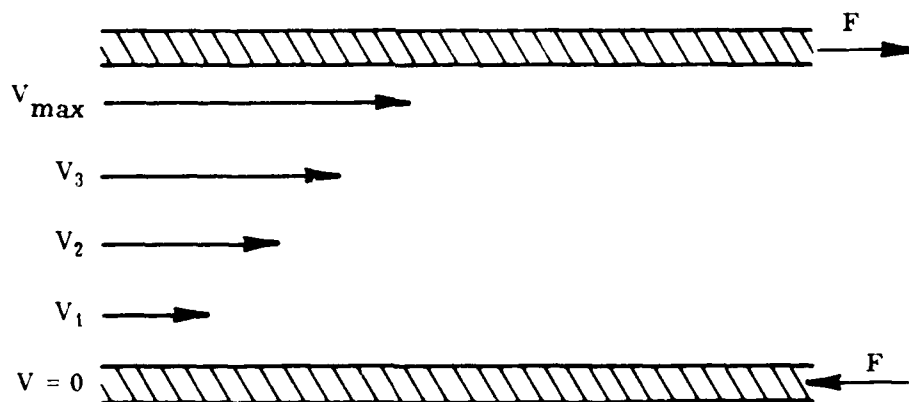


Fig. I-4

Fluids for which μ is not constant but depends on (dV/dZ) are called non-Newtonian.

In metric units, $\mu = \text{dyne sec cm}^{-2} = \text{poise}$

In British units, $\mu = \text{poundal sec ft}^{-2}$

Viscosity is also expressed as centipoise, Cp.

The term "kinematic viscosity" is used when the flow is induced by gravity, as in a vertical capillary tube where the flow is under the liquid's own weight. The expression for kinematic viscosity is $\frac{\mu}{\rho}$, where ρ = density.

$$\text{In metric units, } \frac{\mu}{\rho} = \frac{\text{dyne sec cm}^{-2}}{\text{gm cm}^{-3}} = \frac{\text{gm cm}^{-1} \text{sec}^{-1}}{\text{gm cm}^{-3}} = \frac{\text{cm}^2}{\text{sec}}$$

Fluidity is the reciprocal of viscosity and is identified by the symbol Φ .

The following types of substances are coded for viscosity:

1. All substances in the gaseous state.
2. Liquids of known percent composition and with definite chemical formulas.
3. Fluids of natural substances and their derivatives like milk, wine, beer, blood, peanut oil, etc.
4. Geological materials such as volcanic lava, earth core, sandstone, etc.

The viscosity of the following substances is not coded:

1. The liquid phase of organic compounds. (Includes mixtures containing even one organic compound.)
2. Oxide mixtures (ceramics, glasses, and slags).
3. Oils and lubricants.
4. Polymers.
5. Suspensions (slurries).
6. Non-Newtonian fluids.

The following terms and symbols are coded as viscosity, if clearly defined:

| | | |
|------------------------------|--|-----------------------|
| Absolute viscosity | Kinematic viscosity | Shear viscosity |
| Bulk viscosity | Mean viscosity. | Superfluidity |
| Collision integrals (theory) | Melt viscosity | Viscosity coefficient |
| Dynamic viscosity | η_{sp} ; Relative viscosity (only if value for solvent known) | Volume viscosity |
| Fluidity (Φ) | | |

The following terms are not accepted for coding as property F:

| | | |
|----------------------------|---------------------|---------------------|
| Apparent viscosity | Film coefficient | Solid viscosity |
| Creep | Intrinsic viscosity | Surface viscosity |
| Eddy viscosity of momentum | Magnetic viscosity | Turbulent viscosity |
| | Shear coefficient | Viscoelasticity |

The following list includes uncommon terms related to viscosity which, when encountered, should be brought to the attention of the property consultant to decide if they are codable.

| | | |
|--------------------------|----------------------|----------------------------------|
| Fused viscosity | Pyroscopic viscosity | Viscosity concentration constant |
| Gardner viscosity number | Specific viscosity | Viscosity - gravity constant |
| Inherent viscosity | Structural viscosity | |
| | Transverse viscosity | |

THE THERMAL RADIATIVE PROPERTIES

(G) EMITTANCE, (H) REFLECTANCE, (I) ABSORPTANCE,
(J) TRANSMITTANCE, AND (K) ABSORPTANCE TO
EMITTANCE RATIO

A. The Prime Thermal Radiative Properties (G-J)

The prime thermal radiative properties are emittance, reflectance, absorptance, and transmittance. The latter three obey the law of conservation of energy in the form

$$\alpha + \tau + \rho = 1$$

That is, the energy incident upon the substance is conserved in the form of the absorbed (α), transmitted (τ), and reflected (ρ) fractions. These fractions, dimensionless ratios, are referred to as absorptance, transmittance, and reflectance, respectively. They can be expressed in fractional terms or percentage terms, i. e., from 0 to 1, or 0 to 100%.

Under thermodynamic equilibrium conditions, Kirchhoff's Law is applicable, and the absorbed fraction (α) is equal to the emitted fraction (ϵ); this latter property is called emittance.

These four terms, the so-called prime properties, are further modified by adjectives which are descriptive of the geometric and wavelength conditions, in that order.

Geometric Modifiers* - describe the incidence and/or viewing conditions of the energy

by the use of the terms:

| | |
|------------------|----------------------------|
| angular | diffuse |
| bi-angular | directional |
| bi-conical | hemispherical |
| bi-directional | normal |
| bi-hemispherical | specular |
| bi-normal | total (specular + diffuse) |
| conical | |

Wavelength Modifiers* - describe the portion(s) of the wavelength spectrum in which the energy falls:

| | |
|-----------------|----------|
| heterochromatic | solar |
| integrated | spectral |
| monochromatic | total |

* For a further discussion of many of the geometric and wavelength modifiers, see the Theory, Estimation, and Measurement section in volumes 7, 8, and 9 of the TPRC Data Series.

- Emittance (G) - the ratio of the energy radiated by a substance to the energy radiated by a black body at the same temperature, the comparison being made under the same geometric and wavelength conditions.
- Reflectance (H) - the ratio of the reflected energy to the incident energy; geometric descriptors are used in papers to specify both the incident and reflected beams.
- Absorptance (I) - the ratio of the absorbed energy to the incident energy.
- Transmittance (J) - the ratio of the transmitted energy to the incident energy.

The radiative properties are extremely sensitive to surface conditions of the specimen arising from method of preparation, thermal history, environment, etc. Properties ending in "ivity" are intrinsic properties of the material of which the specimen is composed, and can only be approached by values measured on real specimens that have clean, optically smooth surfaces and are opaque. On the other hand, properties ending in "ance" are the properties of real specimens, regardless of thickness or surface conditions. Hence, the four prime properties are referred to as emittance, reflectance, absorptance, and transmittance.

Frequently optical properties values are measured and stated relative to a standard or known surface. Examples of such standards include freshly smoked magnesium oxide, flowers of sulfur, etc. By knowing the property values of the standard employed, the sample data can be converted to true values.

For reflectance, data obtained by the relative method are referred to as reflectance factor. In most cases there is little numerical difference between (true) reflectance and the reflectance factor since the higher quality standards have reflectance values near unity. Reflectance factor is therefore accepted for coding as property H (reflectivity).

B. Absorptance to Emittance Ratio (K)

The coefficient representing this ratio is frequently described as merely "alpha-over-epsilon" or " α/ϵ ". Like the above prime properties it is specified in papers according to geometric and wavelength conditions.

The most common form of this coefficient is "normal solar absorptance/hemispherical total emittance." It is the ratio of the energy absorbed by a specimen perpendicularly from the sun (or artificial solar source) to that emitted by the specimen into the hemispheric space above the specimen and over all wavelengths. The physical significance of this property is simple: the material with the higher α/ϵ will be the hotter when both are viewing the sun. Consider the situation of a satellite in space, and it follows that its equilibrium temperature will be determined by the value of α/ϵ .

" α/ϵ " can be measured directly by calorimetric techniques where the equilibrium temperature of the specimen is measured when illuminated by a solar source. More commonly found are data generated by indirect methods. The basic principle involves one set of measurements in the wavelength region 0.3 to 2.5 μ of the specimen's normal-hemispherical spectral reflectance $\rho(0, h, \lambda)^*$. The normal solar absorptance is computed by normalizing** $[1-\rho(0, h, \lambda)]$ relative to the wavelength distribution of the solar source (which is approximated by a black body at 5000 K). The hemispherical total emittance is obtained by normalizing $[1-\rho(0, h, \lambda)]$ relative to the wavelength distribution of a black body at the temperature of the specimen (usually in the neighborhood of 300 K). The α/ϵ coefficient follows from the ratio of the two sub-properties computed.

These coefficients calculated by the indirect technique described above are often "hidden" in the text of radiative property documents. Therefore the coder must look for possible α/ϵ values in a paper containing data on the prime radiative properties.

C. Coding Criteria for the Radiative Properties

1. Property Coverage

Related terms for the radiative properties are listed below and are accepted for coding. These properties are coded only when they are expressed in quantitative units, in fractional terms or percentage values. (Bidirectional reflectance is often expressed in steradian units, i.e., ster^{-1} or sr^{-1} . This is accepted for coding, for a steradian is defined as "a unit of measure of solid angles that is expressed as the solid angle subtended at the center of the sphere by a portion of the surface whose area is equal to the square of the radius of the sphere.")

(G) Emittance, ϵ

Degree of blackness (used in Russian papers)
Emissive power
Emissivity

(H) Reflectance, ρ

Albedo
Electroreflectance
Magnetorefectance
Optical reflectivity
Plasma edge reflectivity
Radiance factor

* The symbols within the parentheses indicate the geometric and wavelength conditions: normal (0) incidence, hemispherical (h) viewing, and spectral (λ) wavelength conditions. Note the order: incidence, viewing, and wavelength conditions.

** Normalizing - a mathematical weighting process.

Reflectance factor
 Reflection amplitude
 Reflection coefficient
 Reflection of radiation
 Reflection spectra
 Reflectivity
 Thermoreflectance

(I) Absorptance, α

Absorbance
 Absorptivity
 Absorption spectra (only if the property is clearly defined)
 Infrared spectra (only if the property is clearly defined)

(J) Transmittance, τ

Absorption spectra (only if the property is clearly defined)
 Attenuated total reflectance
 Infrared spectra (only if the property is clearly defined)
 Opacity
 Optical density
 Optical transmittance
 Optical transparency
 Transmission
 Transmission of radiation
 Transmissivity

(K) Absorptance to Emittance Ratio, α/ϵ

Alpha-over-epsilon
 Normal solar absorptance/Hemispherical total emittance
 Solar radiation coefficient

The following terms are not coded for the radiative properties:

| | |
|------------------------|--------------------------|
| Absorbance index | Magnetoreflectance |
| Absorbancy | Molar absorbance index |
| Absorption coefficient | Optical absorption |
| Electroreflectance | Optical property |
| Emission | Transmission (electrons) |
| Emission coefficient | Transmittancy |
| Emittance (ions) | |
| Index of absorption | |

The following types of studies are not coded:

- a. Studies with arbitrary units of scales.
- b. Spectra or band studies - absorption, reflection, and transmission types. These are generally identification methods with property values given in arbitrary units. Even if the units are quantitative, values determined for a qualitative purpose are not coded.
- c. Data expressed in power or energy units, such as energy/area/time, emitted power from black bodies, radiating energy, etc.

2. Wavelength Range

The electromagnetic spectrum (Fig. I-5) embraces a number of ranges: γ -ray, x-ray, ultraviolet, visible, infrared, radar, radio, electrical. The spectrum of interest to TEPIAC is that portion of this total spectrum for

which thermal radiation intensities are significant. Table 15 lists the wavelength ranges of interest in various units. These ranges should only be used as a guide when it is uncertain that a given radiative property is thermal.

THE ELECTROMAGNETIC SPECTRUM

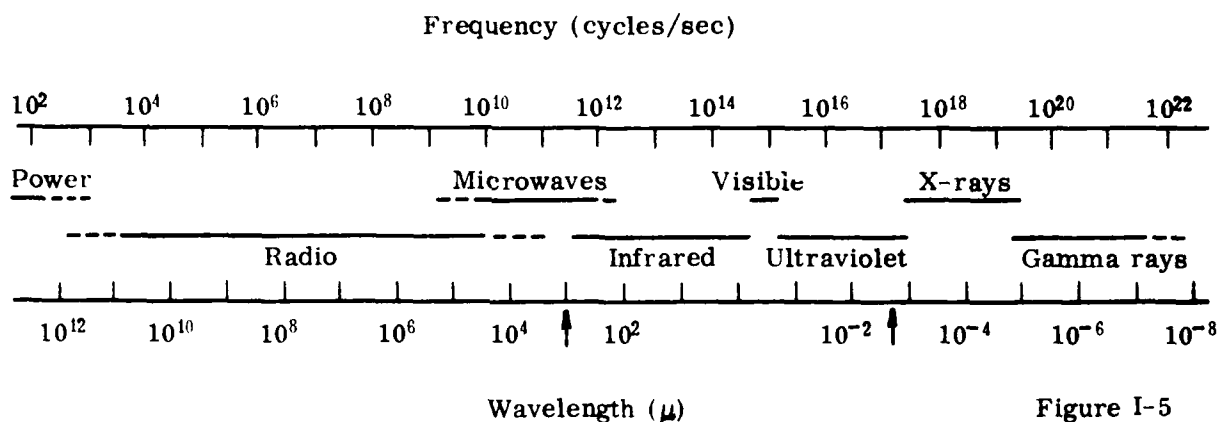


TABLE 15. WAVELENGTH RANGES

| Units | Range | |
|---|-----------------------|-----------------------|
| micron, μ (or micrometer, μm) | 0.05 | 1000 |
| millimicron, $m\mu$ | 50 | 1×10^6 |
| meter, m | 5×10^{-8} | 0.001 |
| centimeter, cm | 5×10^{-6} | 0.1 |
| millimeter, mm | 5×10^{-5} | 1 |
| nanometer, nm | 50 | 1×10^6 |
| angstrom, \AA | 500 | 1×10^7 |
| *wave numbers, cm^{-1} | 2×10^5 | 10 |
| frequency, hertz | 6×10^{15} | 3×10^{11} |
| angular frequency, rad sec^{-1} | 3.77×10^{16} | 1.88×10^{12} |
| electron-volt, eV | 24.8 | 1.24×10^{-3} |

* Sometimes referred to as Kaysers; this unit means the number of waves in a centimeter length. Occasionally, this unit refers to the number of waves times 2π .

3. Substance Coverage

The transmittance and absorptance of liquids, gases, organic substances, inorganic complexes, and adsorbed materials are not accepted for coding. Solids in a KBr pellet or muller with mineral oil, nujol, etc. are coded for the solid, the suspending medium being omitted. For coatings, Class 551, radiative properties for all materials are acceptable.

4. Color

The natural color of a substance is disregarded. An artificially added impurity to induce color is noted as follows:

The color of a substance, if specified in the paper, is noted with the substance entry when coded for radiative properties.

If a substance is artificially colored, but the color is unspecified, then the word "colored" is used.

D. Optical and Thermal Radiative Properties Terminology

$$I_0 = I_a + I_r + I_t,$$

where

I_0 = Incident ray

I_a = Absorbed ray

I_r = Reflected ray

I_t = Transmitted ray

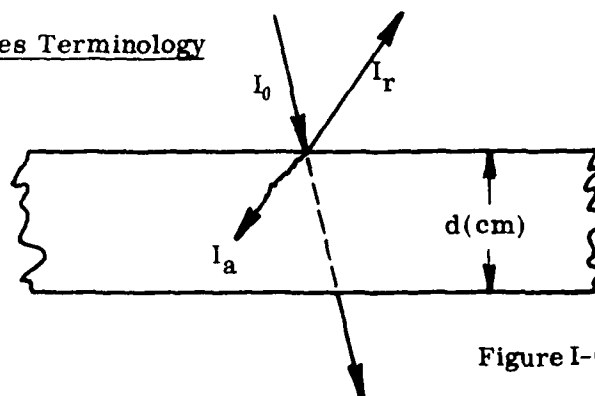


Figure I-6

- *1. Absorbance, A - the logarithm to the base ten of the absorptance, $A < 0$

$$A = \log_{10} \frac{I_a}{I_0} = \log_{10} \alpha$$

Alternate usage: A = logarithm to the base ten of the reciprocal of the transmittance, $A > 0$.
(Coded as transmittance, property J.)

$$A = \log_{10} \frac{I_0}{I_t} = \log_{10} \frac{1}{\tau}$$

2. Absorbance Index, a - is obtained from the relation $A = adc$, where A is the absorbance, d is the thickness, and c is the concentration of the absorbing material.

$$a = \frac{1}{dc} \log_{10} \frac{I_a}{I_0} = \frac{1}{dc} \log_{10} \alpha$$

* Properties with an asterisk are accepted for coding.

Alternate usage: a is obtained from the relation $A = ad$, where A is the absorbance, and d is the thickness.

$$a = \frac{1}{d} \log_{10} \frac{I_a}{I_0} = \frac{1}{d} \log_{10} \alpha$$

3. Absorbancy - the logarithm to the base ten of the transmittancy,

$$= \log_{10} \frac{I_t \text{ (solution)}}{I_t \text{ (solvent)}}$$
- *4. Absorptance, α - the ratio of the radiant flux absorbed in a body of material to the radiant flux incident upon it.

$$\alpha = \frac{I_a}{I_0}$$
- *5. Absorption Spectra - the array of absorption lines and absorption bands which results from the passage of radiant energy from a continuous source through a selectively absorbing medium cooler than the source.
- *6. Absorptivity, α - the absorptance of a specimen that has an optically smooth surface and is thick enough to be opaque.
- *7. Albedo - the fraction of incident light or electromagnetic radiation that is reflected by a surface or body (as the moon, a planet, a cloud, the ground or a field of snow).
8. Complex Dielectric Constant, K^* - expression for the dielectric constant and the relative loss factor. $K^* = \epsilon^*/\epsilon_0 = K' - jK''$, where ϵ^* is the complex permittivity, ϵ_0 is the permittivity of free space, K' is the real dielectric constant (also known as relative permittivity), and K'' is the relative loss factor; the complex dielectric constant is related to the complex index of refraction by $n^* = (K^*)^{\frac{1}{2}}$.
9. Complex Index of Refraction, n^* - expression for the index refraction and index of absorption, $n^* = n \cdot (1 - \kappa) = n - ik$ where κ is the absorption index, n the index of refraction, and k is the index of absorption.
10. Complex Permittivity, ϵ^* - the product of $\epsilon_0 K^*$ where ϵ_0 is the permittivity of free space and K^* is the complex dielectric constant. $\epsilon^* = \epsilon' - i\epsilon''$ where ϵ' is the real permittivity and ϵ'' is the loss factor.
- *11. Electroreflectance - is the reflectance in an electric field.
- *12. Emissivity, ϵ - the emittance of a specimen that has optically smooth surface and is thick enough to be opaque.

- *13. Emittance, ϵ - the ratio of the radiant exitance of a body at a given temperature to that of a blackbody radiator at the same temperature.
14. Index of Absorption, k - the product of the index of refraction, n , and the absorption index, κ , that is $k = n\kappa$.
15. Index of Refraction, n - ratio of the wave (phase) velocity of radiation in a vacuum to velocity of the same radiation in a specified medium.
- *16. Magnetorelectance - is the reflectance in a magnetic field.
17. Molar Absorbance Index - same as absorbance index where b is given in centimeters and c as molar concentration.

$$= \frac{1}{dc} \log_{10} \frac{I_a}{I_0}$$
 where d is in cm and c is the molar concentration.
- *18. Opacity - the reciprocal of the transmission.

$$= \frac{I_0}{I_t}$$
19. Optical Constants - refers specifically to the index of refraction, n , and the absorption index, κ , or the product $n\kappa$.
- *20. Optical Density, D - logarithm to the base ten of the reciprocal of the transmittance (identical to one use of absorbance).

$$D = \log_{10} \frac{I_0}{I_t} = \log_{10} \frac{1}{\tau}$$
21. Optical Properties - collective term embracing primarily optical constants properties, but in many instances inclusive of radiative properties.
- *22. Radiance Factor, β - the ratio of the reflected radiance of a specimen in a given direction under specified conditions of irradiation to that of the ideal, completely reflecting, perfectly diffusing surface, identically irradiated.
- *23. Reflectance, ρ - the ratio of radiant flux reflected from a body to the radiant flux incident upon it.

$$\rho = \frac{I_r}{I_0}$$
- *24. Reflectance Factor, R - the ratio of the flux reflected by a specimen under specified conditions of irradiation and viewing to that reflected by the ideal, completely reflecting, perfectly diffusing surface, identically irradiated and viewed.

*25. Reflectivity, ρ - the reflectance of a specimen that has an optically smooth surface and is thick enough to be opaque.

*26. Transmission - ratio of light flux transmitted to light flux incident; transmittance.

$$= \frac{I_t}{I_0}$$

*27. Transmissivity - transmittance with the effect of surface reflections removed.

*28. Transmittance, τ - ratio of radiant flux transmitted to radiant flux incident.

$$\tau = \frac{I_t}{I_0}$$

29. Transmittancy - ratio of the transmittance of a solution to that of a pure solvent in an equivalent thickness.

$$= \frac{I_t \text{ (solution)}}{I_t \text{ (solvent)}}$$

PRANDTL NUMBER (N)

Prandtl number is a dimensionless ratio that enters into many heat transfer problems involving convection.

The Prandtl number, Pr, or N_{pr} , is a derived quantity defined as the ratio of the molecular diffusivity of momentum (kinematic viscosity), μ/ρ , to the molecular diffusivity of heat (thermal diffusivity), $k/\rho C_p$.

The equation for Pr is:

$$Pr = \frac{C_p \mu}{k} \quad \text{where} \quad \begin{array}{l} C_p = \text{specific heat at} \\ \text{constant pressure} \\ \mu = \text{viscosity} \\ k = \text{thermal conductivity} \end{array} \quad (I-25)$$

The following terms should not be confused with Prandtl number:

Grashof number
Reynolds number
Nusselt number

Elongation percent - This term is accepted only when it is measured under zero stress or strain

Isobaric linear thermal expansion

$\Delta L/L$ vs temperature graph

Lattice constant vs temperature (usually in angstroms)

Lattice parameter linear expansion

Length vs temperature graph

Percent expansion (if linear)

Thermal expansion (if linear)

Thermal linear contraction

THERMAL LINEAR EXPANSION COEFFICIENT (N)

The coefficient of thermal linear expansion is defined as the change in length per unit length of a substance per degree change in temperature (when the temperature of a substance is raised by one degree).

Experimentally it is found that the thermal linear expansion of a solid is proportional to the original length (L_0) at reference temperature T_0 and to the change in temperature (ΔT). Also, it depends upon the nature of the solid material.

Mathematically, this proportionality is represented as follows:

$$L_2 - L_1 \text{ is proportional to } L_0(\Delta T)$$

where $L_2 - L_1$ = difference in the length of solid when heated from temperature T_1 to T_2 .

$$\Delta T = T_2 - T_1.$$

Introducing the proportionality constant, α , the instantaneous coefficient of thermal linear expansion:

$$L_2 - L_1 = \alpha L_0 (\Delta T) \quad (I-26)$$

Thus:

$$\alpha = \frac{L_2 - L_1}{L_0 (\Delta T)} \text{ at } \frac{T_2 + T_1}{2} \quad (I-27)$$

The mean coefficient of thermal linear expansion (from T to T_0) at temperature T is defined as

$$\bar{\alpha}_T = \frac{L_T - L_0}{L_0 (\Delta T)} \quad (I-28)$$

where L_T = length of solid at temperature T

In metric units, $\alpha = \text{cm cm}^{-1} \text{C}^{-1} = \text{C}^{-1}$

In British units, $\alpha = \text{ft ft}^{-1} \text{F}^{-1} = \text{F}^{-1}$

It is important that the units for both linear and volume expansion coefficients are closely examined because the symbols α and β , respectively, are sometimes used interchangeably by authors.

Some of the methods used to measure linear expansion are interferometer, x-ray diffraction, telemicroscope, and dilatometer method.

The following terms are related to and coded as linear expansion:

Diametral expansion
Dilatation

THERMAL VOLUMETRIC EXPANSION COEFFICIENT (β)

The coefficient of thermal volumetric expansion is defined as the change in volume per unit volume of a substance per degree change in temperature (when the temperature of a substance is raised by one degree).

Experimentally, it is found that the thermal volumetric expansion of a solid is proportional to the original volume (V_0) at reference temperature T_0 and to the change in temperature (ΔT). Also, it depends upon the nature of the solid material.

Mathematically, the proportionality is represented as follows:

$$V_2 - V_1 \text{ is proportional to } V_0 (\Delta T)$$

where $V_2 - V_1$ = difference in the volume of a solid when heated from temperature T_1 to T_2 .

$$\Delta T = T_2 - T_1.$$

Introducing the proportionality constant, β , the instantaneous coefficient of thermal volumetric expansion:

$$V_2 - V_1 = \beta V_0 (\Delta T) \quad (I-29)$$

Thus:

$$\beta = \frac{V_2 - V_1}{V_0 (\Delta T)} \text{ at } \frac{T_2 + T_1}{2} \quad (I-30)$$

The mean coefficient of thermal volumetric expansion (from T to T_0) at temperature T is defined as

$$\bar{\beta}_T = \frac{V_T - V_0}{V_0 (\Delta T)} \quad (I-31)$$

where V_T = volume of solid at temperature T .

In metric units, $\beta = \text{cm}^3 \text{ cm}^{-3} \text{ }^\circ\text{C}^{-1} = \text{ }^\circ\text{C}^{-1}$

In British units, $\beta = \text{ft}^3 \text{ ft}^{-3} \text{ }^\circ\text{F}^{-1} = \text{ }^\circ\text{F}^{-1}$

The symbol β is sometimes used interchangeably with the symbol for linear expansion, α ; therefore, the units must always be checked.

If α , β' , and γ are the linear coefficients of expansion in three mutually perpendicular directions, the general relationship connecting these with the coefficient of volume expansion β is:

$$\beta = (1 + \alpha) (1 + \beta') (1 + \gamma) - 1. \quad (I-32)$$

For an isotropic material where $\alpha = \beta' = \gamma$, this reduces to

$$\begin{aligned}\beta &= (1 + \alpha)^3 - 1 = 1 + 3\alpha + 3\alpha^2 + \alpha^3 - 1 \\ &= 3\alpha + 3\alpha^2 + \alpha^3.\end{aligned}\tag{I-33}$$

Neglecting higher order terms

$$\beta \approx 3\alpha.\tag{I-34}$$

Hence, the numerical value of the coefficient of volume expansion is approximately three times that of the coefficient of linear expansion.

The following terms are coded as volume expansion:

- Cubic expansion coefficient
- Cubic lattice constant vs temperature graph
- Density as a function of temperature
- $\Delta\rho/\rho$ as a function of temperature (even one temperature value)
- Isobaric volumetric expansion
- Percent expansion (if volumetric)
- Thermal expansion (if volumetric)
- $\Delta V/V$ vs temperature graph
- Volume vs temperature graph

The following are not coded for volume expansion:

- The Grüneisen constant
- Liquid or gas volume expansion

APPENDIX II
A REVIEW OF THE ELECTRONIC PROPERTIES

TEPIAC investigates the literature for 22 electronic properties. A brief discussion of each property follows.

Throughout this property review, related and unrelated terms are stated as "guide words" to aid the coder in property identification. Property units must always be carefully checked. If there is some doubt as to the advisability of accepting a term as a codable property, the matter should be discussed with a property specialist for a definite decision.

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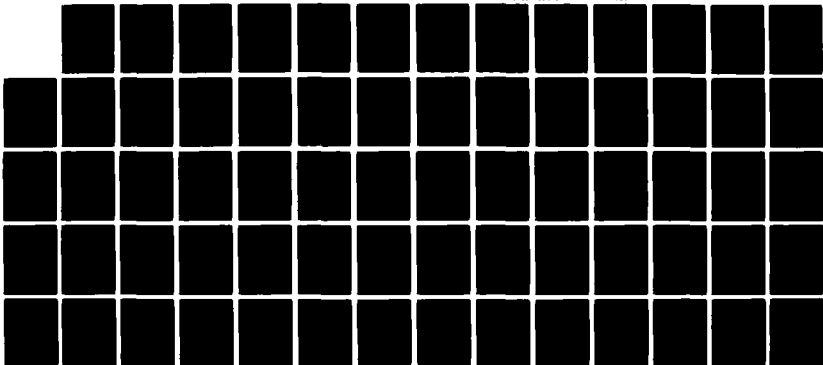
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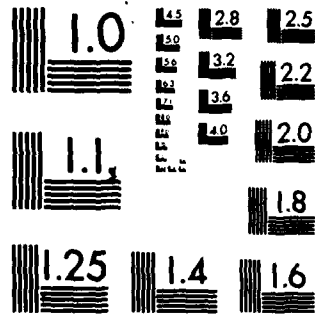
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ABSORPTION COEFFICIENT (AS)

Common Symbols: κ or α

Common Units: cm^{-1} , m^{-1} , db/km (db = decibel)

Defining Equations: $I = I_0 e^{-\alpha x}$
 $I = I_0 (10)^{-\kappa x}$

Definition: When light (or other kind of electromagnetic radiation) penetrates matter, it decreases in intensity. This coefficient, α , is a measure of the rate of decrease, viz., it is a comparison of the intensities of incident and transmitted light, which traverses a medium through a certain distance. The absorption coefficient α is the reciprocal of the thickness required to reduce the intensity to $1/e$ of the incident value (e = base of natural logarithm).

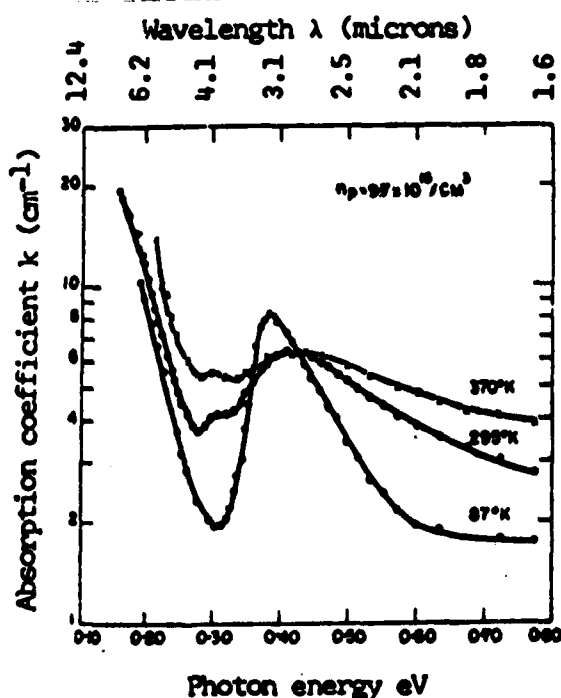


Figure II-1. Absorption Coefficient for Gallium Arsenide. (From EPIC-DS 115.)

Related, Derived, and/or Associated Terms:Acceptable for Coding:

Absorption bands
 Absorption edge
 Absorption index
 Absorption lines
 Absorption spectrum
 Attenuation
 Extinction coefficient

Fundamental absorption edge
 Mass absorption coefficient
 Optical constants
 Optical indices
 Transmission loss
 Urbach's rule
 Volumetric absorption

Borderline Cases: (Codable when clearly related to absorption coefficient)

Absorbance (if thickness of sample given)
 Bouguer's Law
 Bouguer-Lambert Equation
 Kramers-Kronig Analysis
 Optical density (if thickness of sample given)
 Optical properties

Not Acceptable for Coding:

Dispersion
 Fresnel's Equation for Normal Reflectance
 Mass Scattering Coefficient
 Scattering Coefficient
 Volume Scattering Coefficient

Definitions of Related Terms:

Absorption Band or Lines: These are dark bands or lines that appear in absorption spectra, and correspond to more or less narrow frequency ranges in which the incident radiation is relatively strongly absorbed. When the absorption occurs only in narrow frequency ranges, the process may be called selective absorption.

Absorption Edge: A plot of absorption coefficient against wavelength often shows an abrupt change or discontinuity, at a wavelength called an absorption edge. The corresponding energy is the limiting energy for some absorption process, and may be the width of a gap in the energy levels of the absorbing system.

Absorption Index: The quantity k in the complex refractive index $n^* = n - jk$, related to the absorption coefficient α and the wavelength λ of the light by $k = (\lambda\alpha)/4\pi$.

Absorption Spectrum: These spectra show dark regions corresponding to wavelengths for which strong absorption has taken place in a source or transmitting material. They may be classified as continuous, as line spectra, or as band spectra, the last of these being made up of closed and regularly spaced lines.

Attenuation: Is the decrease in light intensity as light traverses a medium, with increasing distance from the source of transmission.

Bouguer's Law: Quantitatively defines the attenuation suffered by a beam of light through absorption and scattering.

Bouguer-Lambert Equation: Defines the absorption coefficient in the absence of scattering.

Extinction Coefficient, k: Is the same as the total absorption coefficient,
 $k = \alpha/2.303.$

Fundamental Absorption Edge: See Absorption Edge.

Kramers-Kronig Analysis: An analysis of the reflection and transmission of light by matter that provides integral relations between the real and imaginary parts of the complex dielectric constant $\epsilon'(\omega) - j\epsilon''(\omega)$, and between the amplitude $R(\omega)$ and the phase angle $\theta(\omega)$ of the complex reflection coefficient. It provides a means for calculating from $R(\omega)$ (known at all frequencies,) the phase angle $\theta(\omega)$; and from these n , k , ϵ' , and ϵ'' at all frequencies.

Mass Absorption Coefficient: This relates the attenuation of light in matter to the mass traversed per unit cross section.

Optical Constants: Refer to some or all of the optical properties, including, but not limited to, the absorption coefficient, refractive index, dielectric constant, etc.

Optical Density: $kd = (\alpha/2.303)d = \log_{10} (I_0/I)$ (where d is distance traveled in sample).

Optical Indices: These are similar to optical constants, and they refer generally to some or all of the optical properties which comprise: refractive index, absorption index, etc.

Optical Properties: The behavior of light in matter, and the indices and coefficients that appear in descriptions of this behavior.

Transmission Loss: Is the loss in energy of the incident light upon traversing a certain medium by a certain distance.

Urbach's Rule: States that near the absorption edge, in many semiconductors, absorption increases exponentially with energy.

Volumetric Absorption Coefficient: Is the volumetric analog of the mass absorption coefficient; it is identical with "absorption coefficient" as defined above.

DIELECTRIC CONSTANT (DC)

Common Symbols: D.C., κ , K , ϵ_r , κ_e , ϵ_0 , ϵ_∞

Common Units: Dimensionless

Defining Equations: $K = \epsilon_r = \epsilon/\epsilon_0$ (for ϵ and ϵ_0 , see below).

$$\kappa_e = \vec{D}/\epsilon_0 \vec{E}$$

Definition: This is the ratio of the capacity of a condenser, having the region between its plates filled with a given dielectric, to the capacity of same condenser, with vacuum in same region.

Related, Derived, and/or Associated Terms:

Acceptable for Coding:

Absolute dielectric constant
Complex dielectric constant
Dielectric coefficient
Dielectric loss
Loss tan δ
Permittivity

Relative capacitance
Relative dielectric constant
Relative permittivity
Specific inductive capacity.
Tan δ

Borderline Cases

Orientation time
Relaxation frequency
Relaxation time

Not Acceptable for Coding:

Dielectric strength
Electric susceptibility
Polarization

Definition of Related Terms:

Dielectric Coefficient: Same as dielectric constant.

Permittivity, ϵ : Is related to permittivity ϵ_0 of empty space (8.85×10^{-12} coulomb²/Newton meter²) by equation $\epsilon = k\epsilon_0$, where k is the relative dielectric constant.

Specific Inductive Capacity: Same as dielectric constant.

DIELECTRIC STRENGTH (DS)

Common Symbols: None

Common Units: V/cm, V/mil

Defining Equation: D. S. = V/m

Definition: Dielectric strength is the maximum electric field a dielectric could withstand without breakdown and subsequent change to a conductor.

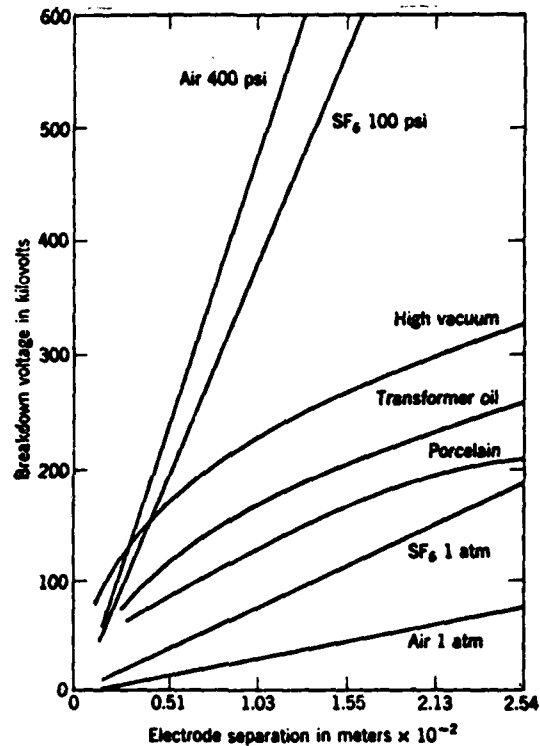


Figure II-2. D-C Breakdown or Dielectric Strength of Various Solids, Liquids, Gases, and Vacuum, in Uniform Fields. Breakdown Voltage versus Dielectric Thickness is Plotted. (From J. Trump, in A. von Hippel, Dielectric Materials and Applications, Wiley, New York, 1954.)

Related, Derived, and/or Associated Terms:

Acceptable for Coding:

Breakdown voltage
 Dielectric breakdown
 Dielectric breakdown voltage
 Disruptive strength
 Electrical strength
 Spark breakdown voltage
 Voltage breakdown

Not Acceptable for Coding:

Dielectric constant
Polarization

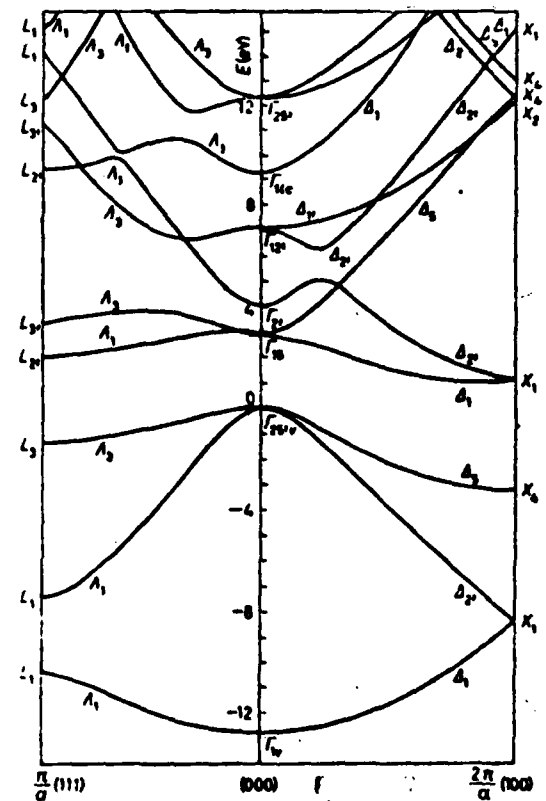
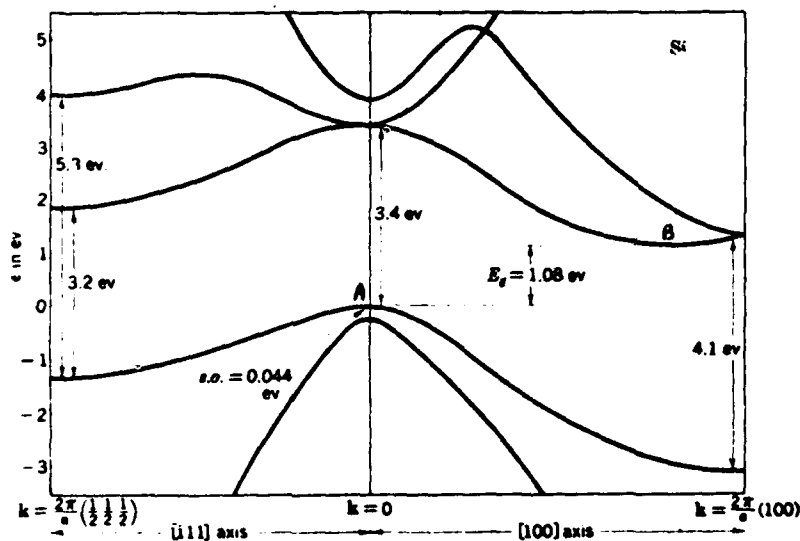
ENERGY BANDS (EB)

Common Symbols: Usually graphical plot

Common Units: None

Definition: Energy band structure is a diagram or representation of the energy bands of range of energy levels assigned to electrons in k space. (See also next page.)

Figure II-3. Calculated Energy Band Structure of Silicon. The Valence Band Edge is at A; the Conduction Band Edge is at B. Spin-Orbit Interaction at $k = 0$ is Shown Exaggerated, it Splits the Valence Band Edge at A by 0.044 eV. The Energy Gap from A to B is 1.08 eV; the Vertical Gap A to C is 3.4 eV. (From Kittel, C., Introduction to Solid State Physics, 1966, and TEPIAC E50507.)



Related, Derived, and/or Associated Terms:

Acceptable for Coding:

Band structure
Conduction band
Valence band

Not Acceptable for Coding:

Energy gap
Energy level
Forbidden band

Definition of Related Terms:

Band Structure: The energy band structure of the solid is the totality of its energy bands. This term is also commonly applied to the detailed dependence of the energy of an electron in the solid on its vector k -value, or to a diagrammatic or analytic representation of this dependence.

Conduction Band(s): In metals, this refers to the bands that are partially filled. In the case of semiconductors or insulators it refers to the lowest bands that are empty at the absolute zero, but are partially occupied by electrons at higher temperatures, or in the presence of impurities or sources of electronic extraction.

Energy Band: An energy band in a crystalline solid is a range of energies that can be assumed by a quasi-free electron in the solid. (There are various refinements of this term.)

Filled Bands: The individual states in a band may be filled (occupied) by an electron, or empty. Bands may be classified as completely filled, partially filled, or empty, according as all, some, or none of the states in the band are filled. Metals have at least one band only partially filled. Semiconductors and insulators have their lowest bands filled, and separated by an energy gap from higher bands that are empty when $T_1 = 0$. In semiconductors this gap is typically small; in insulators it is large (several electron volts or more).

Valence Bands: In non-metals, the highest bands filled with electrons at $T = 0$, which control the binding of atoms or molecules into the crystalline form.

EFFECTIVE MASS (EF)

Common Symbols: m^* , m_e^* , m_h^* , m_p^* , m_n^*

Common Units: Fraction of free electron mass

Definition: Electrons in nearly empty energy bands may contribute to conduction processes as though they were free particles with a different, effective, mass. Unoccupied electron states in nearly filled bands (holes) contribute to conduction processes as though they were free positive carriers with a different effective mass. The effective mass is defined in terms of the acceleration of the carrier produced by an applied field, and can be derived from a detailed specification of the energy band structure. It may have scalar character, or be a tensor, when an applied field does not accelerate the carrier in the same direction as the field.

Related, Derived, and/or Associated Terms:

Acceptable for Coding:

Azbel-Kaner effect
Carrier effective mass
Cyclotron frequency
Cyclotron mass

Cyclotron resonance
Electron effective mass
Hole effective mass

Not Acceptable for Coding:

Interband effects
Intraband effects
Oscillating effect
Zeeman effect

Definition of Related Terms:

Azbel-Kaner Effect: This is a type of cyclotron resonance in high purity metals at liquid helium temperatures, which could be used to measure effective masses of carriers.

Cyclotron Resonance: The quasi-free carriers in a material, when subject to a fixed magnetic field and an oscillating electromagnetic field, exhibit a resonance analogous to that in a cyclotron when the oscillating field has the appropriate resonant frequency. This becomes evident in the strong absorption of the electromagnetic radiation by the material, and can be used to determine the effective mass of the carriers.

ENERGY GAP (EG)

Common Symbol: E_g

Common Unit: eV

Defining Equations: $E_g = kT \ln(\rho/A)$
 $E_g = \Delta R / \Delta T$

Definition: This is the difference in energy between the highest state in the valence band and the lowest state in the conduction band. (See Energy Band figure caption, page 92).

Depending on the size of this gap, materials are classified into metals, semiconductors, and insulators.

This energy gap may vary with pressure, electric, and magnetic fields.

Metals have the lowest energy gaps, then semiconductors, and then insulators.

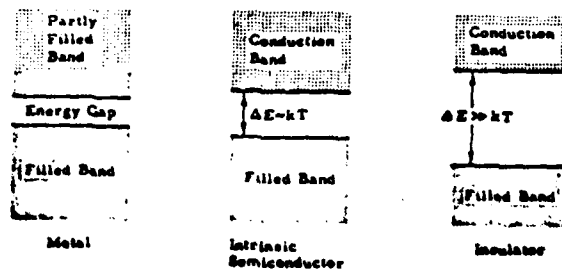


Figure II-4. Effects of Width of Energy Gap and Level of Filled Energy States in Determining Conductivity Characteristics for Insulators, Semiconductors, and Conductors. (From Rose, R. M., Shepard, L. A., Wulff, J., The Structure and Properties of Materials, Vol. IV: Electronic Properties.)

Related, Derived, and/or Associated Terms:

Acceptable for Coding:

Absorption band edge
 Activation energy
 Band gap
 Forbidden energy band
 Intrinsic ionization energy
 Superconductive energy gap

Definitions of Related Terms:

Absorption Band Edge: Discussed under the section of "Absorption Coefficient" (page 86).

Activation Energy: Is the energy required to make possible some transport process (or other phenomenon).

In the case of electrical conduction in an intrinsic semiconductor, it is necessary that electrons be excited from the valence band to the conduction band, by adding an energy at least equal to the energy gap. The energy gap is commonly determined, using the approximate relation

$$\ln \rho(T) = A + \frac{E_g}{kT},$$

from the slope of a plot of the logarithm of electrical resistivity ρ against $1/T$.

Band Gap: Same as energy gap.

Forbidden Energy Band: Same as energy gap.

Intrinsic Ionization (Activation) Energy: Is the activation energy for electrical conduction in a pure material, as distinguished from the lower activation energy for conduction that may arise from the presence of impurities.

Superconductive Energy Gap: Is the energy gap of the material near its superconductive state.

ELECTRICAL HYSTERESIS (EH)

Definition: This is a phenomenon whereby the actual electric polarization of a dielectric substance depends not only on the existing electrical intensity, but on its previous electrical state as well. This results in dissipation of energy (the dielectric hysteresis loss), when the substance is subjected to an alternating electric field.

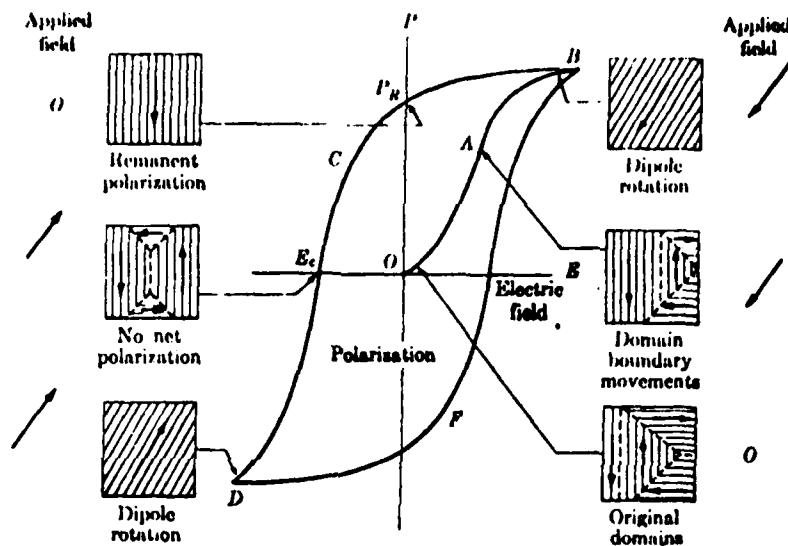


Figure II-5. Electric Hysteresis Loop. (From TEPIAC Final Report, Jan. 1974.)

Related, Derived, and/or Associated Terms:

Acceptable for Coding:

Coercive field
 Dielectric absorption
 Dielectric hysteresis loop
 Dielectric susceptibility
 Differential susceptibility
 Electric domains
 Ferroelectric(-ity)

Ferroelectric Curie temperature
 Ferroelectric domains
 Initial polarization curve
 Initial susceptibility
 Remanent polarization
 Saturation susceptibility

Not Acceptable for Coding

Curie temperature (magnetic)

Definition of Related Terms:

Coercive Field: The magnitude of the reversed electric field E_c required to bring the polarization back to 0.

Dielectric Absorption: Same as electrical hysteresis.

Dielectric Hysteresis Loop: Same as hysteresis loop.

Dielectric Susceptibility: Is the degree of susceptibility to polarization, when an electric field is applied, measured by the ratio of the polarization to the field that produces it.

Differential Susceptibility: Is the susceptibility at various points on the hysteresis loop, as measured by the slope of the loop.

Electric Domain: Is a small region of material where all the electric dipole moments are aligned.

Ferroelectric: Is a substance which has a spontaneous polarization reversible by an applied electric field.

Hysteresis Loop: Is the curve showing the relation between the polarization and the electric field.

Polarization: Is the total dipole moment which occurs within and on the surfaces of the dielectric.

Remanent Polarization: The polarization P_R that remains when the electric field returns to 0.

Saturation Polarization: The polarization of a material approaches a maximum "saturation" value as the inducing field becomes very large.

Saturation Susceptibility: This term is sometimes loosely used as a synonym for saturation polarization. Strictly, defined as a ratio of polarization to field, susceptibility would go to zero as the field becomes very large.

ENERGY LEVEL (EL)

Common Symbols: None

Common Units: eV

Definition: Energy level is a well-defined energy state (of a certain allowable value) where electrons in atoms and molecules exist. These levels are indicated by lines. When an electron changes its energy by changing state, the energy is emitted or absorbed in the form of a photon, of a specific frequency, obeying the energy change equation.

The higher the atomic number, the more complex the atom is, and hence the greater the number of its filled energy levels is. Molecules are far more complicated than atoms and have a greater number of levels because an electron here would be subjected to the fields of multiple nuclei, and hence many transitions are possible.

There are two types of energy levels which are coded. Atomic or molecular energy level is identified by physical state code "ionized" and code parameter "I". The electronic energy level (usually level within the energy gap) usually has physical state codes "doped", "solid", or "thick or thin film".

Related, Derived, and/or Associated Terms:

Acceptable for Coding:

| | | |
|--------------------|---------------------|-----------------|
| Acceptor levels | Equi-energy surface | Quantum level |
| Chemical potential | Exciton levels | Quantum numbers |
| Degenerate levels | Fermi level | Stark levels |
| Donor levels | Fermi surface | Surface state |
| Energy contours | Ionization energy | Trap |
| Energy state | Landau levels | |

Not Acceptable for Coding:

Density of states
Energy bands
Energy gaps
Eigenfunction
Eigenvalue

Definitions of Related Terms:

Acceptor Levels: These are energy levels lying in the vicinity of the valence band, of electrons trapped near acceptor impurities.

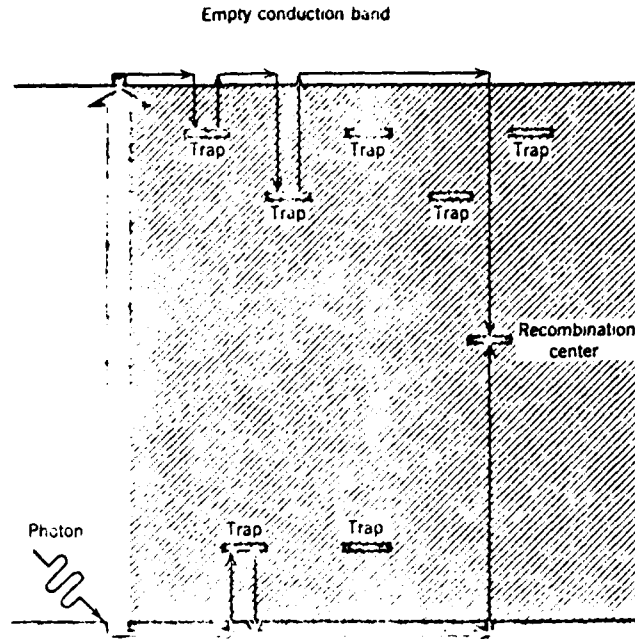


Figure II-6. Electronic Energy Levels. Generation, Trapping, and Recombination of Excess Minority Carriers. (From Rose, R. M., Shepard, L. A., Wulff, J., The Structure and Properties of Materials, Vol. IV: Electronic Properties.)

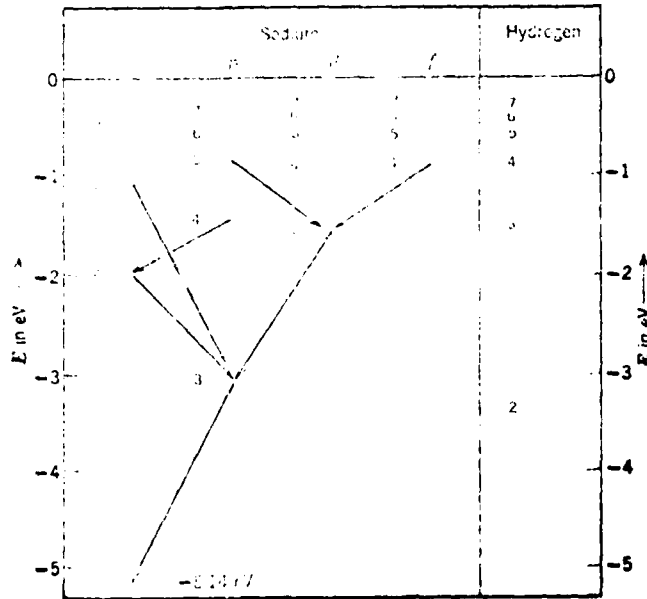


Figure II-7. Atomic Energy Level. The Energy Level Diagram for Atomic Sodium. (From Rose, R. M., Shepard, L. A., Wulff, J., The Structure and Properties of Materials, Vol. IV: Electronic Properties.)

Chemical Potential: In a complex system the chemical potential of a component is the change in free energy, per mole of that component. In chemistry it plays an important role in the discussion of reactions. In crystal physics, the chemical potential per electron appears as the Fermi energy.

Degenerate Levels: Are two states or levels having the same energy values.

Donor Levels: These are energy levels, lying in the vicinity of the conduction band, of electrons trapped in the vicinity of the donor atom.

Energy Contours: In illustrating the dependence of energy on other physical parameters, one may present energy contours, or lines of equal energy, in diagrams in which the other variables appear as coordinates.

Energy States: Different states, associated with different energy values.

Equi-Energy Surface: When energy contours are plotted in three dimensions, the result is a surface having the same energy value at all its points.

Exciton Levels: Energy levels associated with localized electronic excitations in a solid, such as excitations of single molecules in a molecular crystal, or of an electron-hole pair in a semiconductor.

Fermi Level (or Fermi Energy): This is the energy of the highest filled electron states in a metal at 0 °K.

Fermi Surface: Is the surface in k-space corresponding to states with the Fermi energy.

Ionization Energy: Is the minimum energy or potential through which an electron must have fallen in order to ionize an atom or molecule of a specific substance. It is the energy required to remove an electron from an atom or molecule to an infinite distance.

Landau Levels: Certain discrete energy levels for carriers moving in a periodic potential plus a uniform magnetic field.

Quantum Level: Is an energy level associated with a particular quantum number.

Quantum Numbers: Are numbers designating the various energy levels, e.g., quantum number $n = 1$ corresponds to the lowest energy state of the electron in a hydrogen atom.

Stark Levels: Are the energy levels that arise when a source is subjected to a strong electric field which splits and polarizes its spectral lines.

Surface States: These are discrete energy levels produced by surface imperfections.

Trap: Is an energy level that can capture either electrons or holes easily, but not both.

ELECTRICAL RESISTIVITY AND CONDUCTIVITY (ER)

Common Symbols: ρ, σ

Common Units: $\text{ohm}^{-1} \text{cm}^{-1}$; mho/cm; mho/m; $\text{ohm}\cdot\text{m}$; $\mu\Omega\text{-cm}$; $\Omega\text{-cm}$; $\Omega\cdot\text{m}$; $\Omega\cdot\text{c mil/ft}$; $\Omega\text{-in}$; $\Omega\text{-ft}$; $\text{cm}\mu$; $\text{es}\mu$; $\Omega\text{-mm}^2/\text{m}$; % IACS; $\frac{\Omega/\square}{\text{cm}}$

Defining Equation: $\rho_{ik} = \frac{\vec{E}_k}{\vec{j}_i}, \rho = \frac{A}{\Delta X} R$

Definition: This is the ratio of the electrical current density flowing to the applied electrical field strength. It is a measure of the conductance of or resistance to current flow by a substance. In this respect, materials are classified into three categories, depending upon their resistances and also the functional dependence of these resistance on temperature:

- Metals: Here resistivity is relatively low and temperature coefficient is usually positive.
- Semiconductors: Here the temperature coefficient of resistivity is negative and may be quite large. The magnitude of the resistivity is sensitive to the presence of impurities. Controlled addition of small amounts of other materials (doping) is commonly employed to achieve desired characteristics for the electrical resistivity.
- Insulators: Conductivities here are very low. This group includes many hydrocarbons, other organic materials, and covalently bonded lattices.

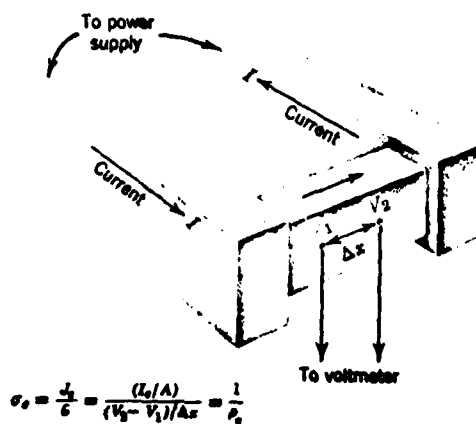


Figure II-8. Measurement of Electrical Conductivity of a Specimen of Cross-Sectional Area A. (From Rose, R. M., Shepard, L. A., Wulff, J., The Structure and Properties of Materials, Vol. IV: Electronic Properties.)

Related, Derived, and/or Associated Terms:Acceptable for Coding:

Conductivity
 Electrical resistance (as a function of temperature)
 Electrical resistivity
 Piezoresistance
 $\Delta\rho/\Delta P$ (variation of resistivity with pressure)
 $\Delta\rho/\Delta T$ (variation of resistivity with temperature)
 RRR (residual resistance ratio)
 $R_{273^\circ\text{C}}/R_t$
 Resistivity
 Specific conductance
 Specific resistance
 Superconductivity transition temperature

Borderline Cases:

Kondo temperature
 Lorenz number
 Lorenz-Sommerfeld Rule
 Mean free path
 Mean free time
 Sheet resistivity (when thickness is known)

Not Acceptable for Coding:

Activation energy
 Carrier concentration
 Electrical contact resistance

Definition of Related Terms:

Conductivity, σ : Is the ability of a substance to allow current to pass through it. It is the opposite and inverse of resistivity.

Electrical Resistance, R: Is the total resistance offered by substance as a whole to current flow - unlike resistivity, ρ , which is the amount per a specified unit only of substance, $R = \frac{l}{A} \rho$.

IACS: International Annealed Copper Standard. 100% IACS = $1/58 \Omega \text{mm}^2/\text{m}$ at 20°C (p. 76 of E101316).

Piezoresistance: Is the resistance change effected while subjecting a substance to pressure or stress.

Superconductive Transition Temperature: Is the temperature at or below which a substance becomes a superconductor, with its conductivity tending to infinity (viz., zero resistivity). These temperatures are usually very low, of the order of a few $^\circ\text{K}$.

HALL COEFFICIENT (HC)

Common Symbols: R_H , R , A_H

Common Units: $\text{m}^3/\text{Coulomb}$, $\text{cm}^3/\text{Coulomb}$, $\text{V} \cdot \text{m}^3 \cdot \text{A}^{-1} \text{W}^{-1}$

Defining Equations: $R_H = \frac{E_z}{B_y J_x}$

$\text{V} \cdot \text{cm} \cdot \text{A}^{-1} \cdot \text{G} \text{ s}^{-1}$

Definition: When a magnetic field is applied perpendicular to a current passing through a metal or semiconductor, there appears a potential difference across the conductor perpendicular to both the current and the applied magnetic field. This is the Hall Effect, of which the Hall Constant is a measure.

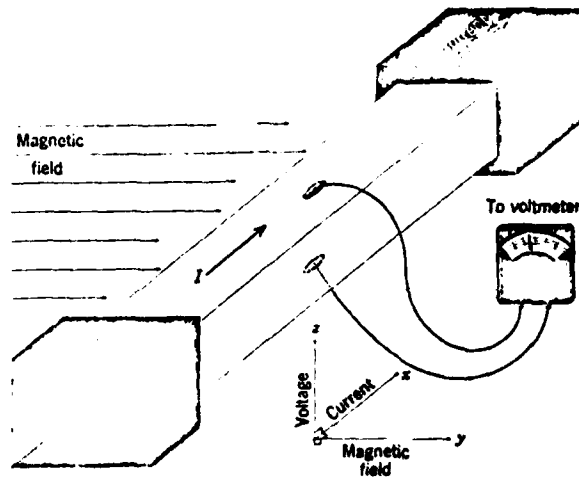


Figure II-9. Measurement of the Hall Effect. The Directions of the Applied Magnetic Field, Electric Current, and Hall Voltage are Mutually Perpendicular. (From Rose, R. M., Shepard, L. A., Wulff, J., The Structure and Properties of Materials, Vol. IV: Electronic Properties.)

Related, Derived, and/or Associated Terms:

Acceptable for Coding:

Corbino effect
Hall carriers
Hall effect

Hall e. m. f.
Hall resistivity
Hall voltage

Not Acceptable for Coding:

Extraordinary Hall coefficient
Longitudinal Hall effect

Definition of Related Terms:

Corbino Effect: Is a special case of Hall Effect. Here, a circular disk is considered with current flowing radially and placed perpendicular to a magnetic field. In this case, a component of the current flows around the disk.

Hall Carriers: Are the charge carriers in semiconductors, undergoing the Hall Effect. The sign of the Hall Constant indicates the sign of the dominant carriers, and its magnitude provides important information about the concentrations of the carriers, though it does not uniquely determine these concentrations.

Hall e. m. f.: Same as Hall voltage.

Hall Resistivity: Is the resistivity of the material undergoing Hall Effect.

Hall Voltage: Is the potential that arises when a material is undergoing the Hall Effect.

MAGNETIC HYSTERESIS (MH)

Common Symbols: B_m , H_m , H_c , B_r , P_h , $B-H_{max}$

Common Units: Oersteds, gauss, ergs/cm³/cycle, gauss-oersteds

Defining Equation: $B = H + 4\pi M$

Definition: This is the phenomenon depicted by a ferromagnetic material in which the magnetic induction does not only depend on the existing magnetic field strength, but also on the previous condition of the substance.

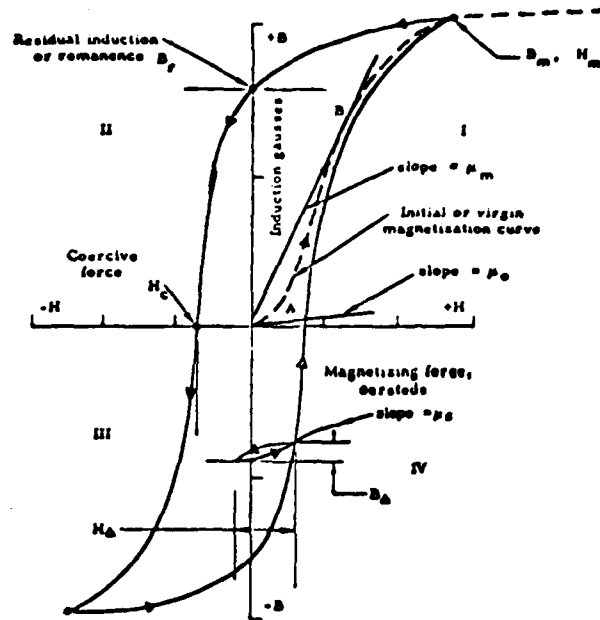


Figure II-10. Magnetic Hysteresis Curve. (From EPIC-S7.)

Related, Derived, and/or Associated Terms:

Acceptable for Coding:

Barkhausen effect
 Barkhausen jumps
 Coercive force
 Coercivity
 Demagnetization curve
 Energy product $B-H_{max}$
 Ferrimagnetic domains
 Ferromagnetic domains

Hysteresis loss
 Initial magnetization curve
 Initial permeability
 Magnetic domains
 Magnetic hysteresis
 Magnetic hysteresis loop
 Maximum permeability
 Remanence

Not Acceptable for Coding:

Antiferromagnetism
 Asymptotic Curie temperature
 Curie constant
 Curie law
 Curie temperature
 Curie-Weiss law
 Diamagnetism

Ferromagnetic Curie point
 de Haas-van Alphen effect
 Magnetic moment
 Mass susceptibility
 Molar susceptibility
 Néel temperature
 Paramagnetism

Definition of Related Terms:

Barkhausen Effect: Sudden small changes in the magnetization of a ferromagnet due to Barkhausen Jumps.

Barkhausen Jumps: Sudden changes in the magnetization of individual domains in a magnet.

Coercive Force: Is the reversed magnetic field strength needed to reduce the magnetic induction to zero.

Energy Product $B-H_{\max}$: This is a measure of the usefulness of a magnet. It is twice the maximum magnetic potential energy of the magnet.

Ferrimagnetic and Ferromagnetic Domains: Small regions in a magnet with uniform spontaneous magnetization. The magnetization of the magnets as a whole is the resultant of the domain magnetizations, and changes during a hysteresis cycle because the orientation and volume of the magnetic domains varies, even though the magnitude of their magnetic moment per unit volume remains constant.

MOBILITY (MO)

Common Symbol: μ

Common Units: $\text{cm}^2/\text{V-sec}$, $\text{m}^2/\text{V-sec}$

Defining Equations: $\mu = \sigma/en$, $\mu_H = R_H\sigma$

Definition: Mobility is the magnitude of the average drift velocity of a charged carrier per unit electrical field applied. The charged carriers may be electrons, holes or ions, and the associated mobilities are referred to as electron, hole and ionic mobilities. In semiconductors both holes and electrons are present, and it is common to refer to the mobilities of majority carriers and of minority carriers.

Related, Derived, and/or Associated Terms:

Acceptable for Coding:

Conductivity mobility
Diffusivity-mobility ratio
Drift mobility
Drift velocity
Electron mobility

Hall mobility
Hole mobility
Ionic mobility
Mobility

Definition of Related Terms:

Conductivity Mobility: Is the mobility deduced from conductivity and carrier concentration.

Drift Mobility: Is the mobility determined from direct observation of the drift of a pulse of injected minority carriers. If minority carrier concentration is small with respect to that of the majority carriers, the drift mobility equals the conductivity mobility of the minority carriers.

Hall Mobility, μ_H : Is the mobility deduced from Hall effect measurements and a simple approximate theory.

MAGNETIC SUSCEPTIBILITY (MS)

Common Symbols: χ , χ_m

Common Units: Dimensionless but will find in use: $\text{cm}^3 \cdot \text{gm}^{-1}$, $\text{m}^3 \text{mol}^{-1}$

Defining Equation: $\chi_m = \frac{M}{H} = \mu_r - 1 = \frac{\mu - \mu_0}{\mu_0}$

Definition: Magnetic susceptibility is the magnetic dipole moment induced in a material by unit magnetic field.

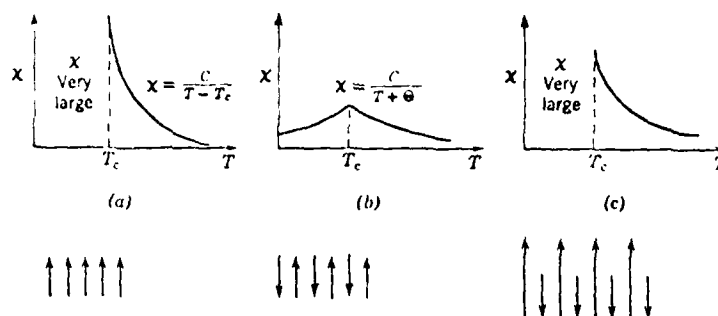


Figure II-11. Magnetic Susceptibility versus T for (a) Ferromagnetic, (b) Antiferromagnetic, and (c) Ferrimagnetic Materials, with Magnetic Moment Alignments Indicated for Each Case. (From Rose, R. M., Shepard, L. A., Wulff, J., The Structure and Properties of Materials, Vol. IV: Electronic Properties.)

Related, Derived, and/or Associated Terms:

Acceptable for Coding:

Antiferromagnetism
Asymptotic Curie temperature
Curie constant
Curie law
Curie temperature
Curie-Weiss law
Diamagnetism
Ferromagnetic Curie point
Ferromagnetic Curie temperature

de Haas-van Alphen effect
Inverse magnetic susceptibility
Magnetic moment
Magnetic transition temperature
Mass susceptibility
Molar susceptibility
Néel temperature
Paramagnetism
Weiss constant

Not Acceptable for Coding:

Barkhausen effect
Barkhausen jumps
Coercive force
Demagnetization curve
Hysteresis loss
Initial magnetization curve
Initial permeability

Magnetic domain
Magnetic hysteresis
Magnetic hysteresis loop
Magnetization
Maximum permeability
Remanence

Definition of Related Terms:

Anti-Ferromagnetism: Below a temperature known as the Néel Temperature, T_N , some materials exhibit spontaneous magnetization of two magnetic sublattices with equal moments oppositely aligned. The result is strong magnetic ordering on the atomic scale, but with zero net magnetization.

Curie Temperature: This is the critical temperature, T_C , below which ferromagnetic materials experience the onset of a spontaneous magnetization (in a zero applied magnetic field).

Above this T_C , the material is paramagnetic. At this T_C , there is an order-disorder transition in the alignment of magnetic moments or induced electric dipoles in a solid.

Diamagnetism: This is the phenomenon observed when a magnetic field is applied to a material, whereby the electron motion in the individual atoms is slightly modified by the magnetic force exerted upon the moving charges.

Such modified motion of the electrons in turn gives rise to a negative induced magnetic moment, opposing the applied field.

Ferrimagnetism: Pertains to materials having two sets of magnetic moments, oppositely directed but differing in magnitude. Hence, there is a resultant net magnetization, less than that of either sublattice.

Ferromagnetism: Is exhibited by materials, characterized by the onset of a spontaneous magnetization (in a zero applied field) below a certain critical temperature, T_C , known commonly as the Curie temperature.

de Haas-van Alphen Effect: This is the oscillatory dependence of the diamagnetic susceptibility of the charge carriers of many metals on magnetic field.

This effect is due to the quantization of electron orbits placed in a magnetic field, and is more pronounced with large magnetic fields, low temperatures and small effective masses.

Néel Temperature: This is the critical temperature, T_N , below which antiferromagnets show spontaneous sublattice magnetization but zero net magnetization. Above T_N these materials are paramagnetic.

Paramagnetism: Is observed in materials in which the individual atoms have a magnetic moment. The magnetic dipole here, will align with the applied magnetic field, thus producing a positive induced magnetic moment.

Remarks

To distinguish better between Magnetic Susceptibility and Magnetic Hysteresis, the following points should be borne in mind by the coder:

Ferromagnetic and Ferrimagnetic Materials: In the graph of χ_m vs. T, for values of T equal to or above T_c , the property will be Magnetic Susceptibility.

Below T_c , the property is Magnetic Hysteresis.

Also when $\chi_m \rightarrow \infty$, it is Magnetic Hysteresis.

Antiferromagnetic Materials: The entire region of the curve χ_m vs. T, pertains to the property Magnetic Susceptibility. This includes temperatures below and above T_N , and at T_N .

Hysteresis Loop, and all closely connected characteristics on it, such as the initial magnetization curve and the Barkhausen effect and jumps, pertains to Magnetic Hysteresis.

REFRACTIVE INDEX (RI)

Common Symbol: n

Common Units: None (Dimensionless)

Defining Equation: $n = \frac{c}{v}$

Definition: The refractive index is the ratio of the phase velocity of light, which is an electromagnetic radiation, in vacuum, to its phase velocity in a specific medium.

It is a function of both the wavelength of the incident light, and the molecular structure and orientation of the medium.

Related, Derived or Associated Terms:

Acceptable for Coding:

| | |
|---|---|
| Birefringence | Fresnel's equation for normal reflectance |
| Complex index of refraction | Index of refraction |
| Dispersion | Kramers-Kronig Analysis |
| Double refraction | Kronig-Kramers Analysis |
| dn/dP (index variation with pressure) | Optical dispersion |
| dn/dT (index variation with temperature) | Optical polarization |
| $dn/d\lambda$ (index variation with wavelength) | Ordinary ray or wave |
| Elasto-optic constants | Piezooptics |
| Extraordinary ray or wave | Stress coefficient |

Definition of Related Terms:

Birefringence: In highly symmetric (cubic) crystals, the refractive index is independent of the polarization and directions of the transmitted light, and there is a single refractive index $n(w)$. All non-cubic crystals show some (usually small) deviation from this simple behavior. A beam of light incident on these crystals will usually be split into two, with different directions of propagation and different characteristic polarizations. A light pulse emitted by a point source within such a crystal will be propagated outward with two wave fronts, one or both of which will be non-spherical, and the wave polarization will vary in a characteristic way over each wave surface. This phenomenon is called birefringence, since two refractive indices are required to describe the propagation of light in each direction.

In an uniaxial crystal one of the two waves spreading from a point source in the crystal will be spherical, the other ellipsoidal. These are referred to as the ordinary and extraordinary waves, respectively. A light beam incident normally on a plane slab of a uniaxial crystal will be split into an

ordinary ray, which will emerge without lateral deviation, and an extraordinary ray, which will give rise to an emergent ray parallel to the incident ray, but laterally displaced. For biaxial crystals it is necessary to specify three principal refractive indices.

Dispersion: Variation of the velocity of propagation of light, in a solid, is a function of frequency.

Double Refraction: Same as Birefringence.

dn/dT , dn/dP , $dn/d\lambda$: Show the functional dependence or variation of the refractive index on temperature, pressure and wavelength respectively.

Extraordinary Ray, Beam or Wave: See Birefringence.

Fresnel's Equation for Normal Reflectance: Is an equation that is employed to compute refractive indices.

Kramers-Kronig Analysis: See page 87.

Optical Polarization: This is the process whereby the vibrations of light or other transverse wave radiations are confined to a single plane (linear or planar polarization), or confined to two mutually perpendicular planes with the components having a particular relationship between their phases and amplitudes (circular or elliptical polarization).

Ordinary Ray, Beam or Wave: See Birefringence.

Piezooptics: Deals with the effects of pressure or stress, applied to a crystal, on the refractive index.

Stress Coefficient: Indicates the variation of refractive index with stress on the material.

WORK FUNCTION (WF)

Common Symbol: E_w

Common Unit: eV

Defining Equation: $E_w = \chi - E_F$

Definition: This is the minimum additional energy that an electron inside a metal has to be given, to enable it to escape to the outside vacuum, at 0 °K.

Related, Derived and/or Associated Terms:

Acceptable for Coding:

Electron Affinity
External Work Function
Internal Work Function

Definition of Related Terms:

Electron Affinity: Is the energy difference between the bottom of the conduction band and the vacuum level (the energy of an electron at rest outside the solid). It is the work needed to remove the electron to infinity, from the conduction band.

External Work Function: Same as electron affinity.

Internal Work Function: Is the energy difference between the bottom of the conduction band and the Fermi level.

Remarks:

When the work function of a thin layer of one material on another material is reported, system class material directory entries are avoided. Instead, code for physical state thin film, T, for the top material and solid, S, for the bottom material.

ELECTRON EMISSION PROPERTIES (EP)

Common Symbols: See below

Common Units: See below

Defining Equations: $J = AT^2 \exp(-E_W/kT)$

$$J = A_F E^2 \exp(-B/E)$$

$$J = AT^2 f(E_M/kT)$$

Definition: Electron emission includes a variety of processes whereby electrons escape from the surface of a solid, or other material.

In all such cases, the electron requires sufficient energy to escape from the surface, to distances up to several hundred atomic diameters from the surface, in which location the electron is considered to be free.

If electrons leave the material because of its high temperatures, the phenomenon is Electron Thermionic Emission. If energetic particles are employed to bombard the material, and hence induce electron escape from the surface, then the process is termed Electron Secondary Emission.

If the causant is a strong electrical field, used to pull electrons out of the material surface, then the process is known as Electron Field Emission.

If photons provide the energy required for the electrons to leave the surface, the process is Electron Photoemission.

Still, in all these processes, the entity emitted is an Electron.

A. Thermionic Emission:

Common Symbols: J (Electron Current Density)

Common Units: A/m²

Definition: This is a subcategory, as mentioned earlier, of Electron Emission, in which electrons leave the heated surface of materials.

Related, Derived and/or Associated Terms:

Dushman-Richardson equation
Edison Effect
Electron thermionic emission
Exoemission
Richardson's Constant
Richardson-Dushman equation
Richardson's Effect
Richardson Equation
Richardson Lines

Richardson plot
Saturated current density
Saturated emission
Schottky Effect
Schottky Line
Schottky Plot
Thermal electron emission
Thermionic electron emission
Transmission coefficient

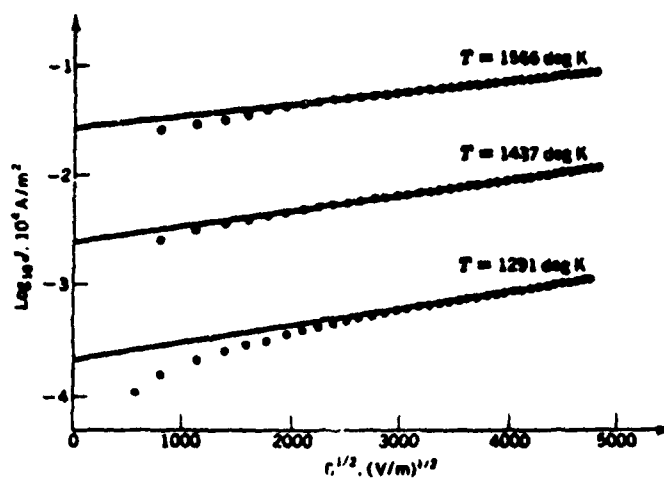


Figure II-12. Schottky Plots. (From TEPIAC Final Report, January 1974.)

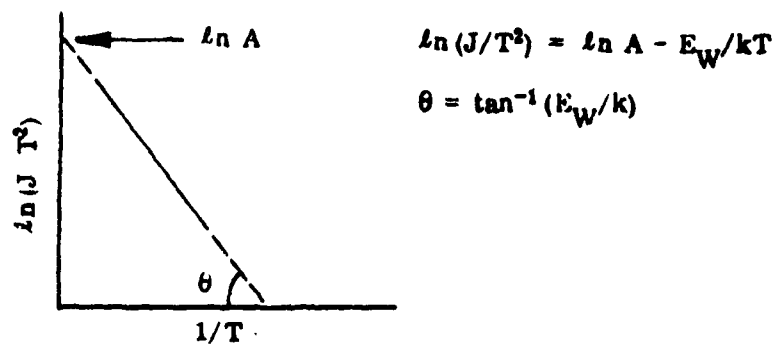


Figure II-13. Richardson Plot. (From TEPIAC Final Report, January 1974.)

Definitions of Related Terms:

Dushman-Richardson Equation: Similar to Richardson Equation.

Edison Effect: This is another name for thermionic emission.

Electron Thermionic Emission: An alternate term for Thermionic Emission.

Exoemission: Same as thermionic emission.

Richardson Equation: Describes the thermionic emission as a function of T.

Richardson Lines, Plots, Constant and Effect: All relate to thermionic emission of a metal. See Figure II-13 for illustration.

Saturated Current Density: Is the current density obtained when saturated emission takes place - where all emitted electrons are collected.

Saturated Emission: Occurs when all emitted electrons are collected, and a build-up of a substantial space charge above the surface is prevented.

Schottky Effect: Is the application of an electric field to help lower the work function of electrons ready to leave the surface but hindered by a space charge already formed around the heated surface.

Schottky Line, Plot: These depict the Schottky Effect quantitatively. See Figure II-12.

Thermal or Thermionic Electron Emission: Other commonly used variants of the name for Thermionic Emission.

Transmission Coefficient: Is a measure of the probability that an electron with energy sufficient to cross the surface barrier will in fact go through the surface.

B. Field Emission:

Common Symbols: J (Electron Current Density)

Common Units: A/m²

Definition: This is also a subcategory of Electron Emission in which the emission or escape of electrons through the metal or semiconductor surface is due to the presence of a strong electric field.

Related, Derived and/or Associated Terms:Acceptable for Coding:

Cold emission
 Electron field emission
 Field emission

Fowler-Nordheim Equation
 Fowler-Nordheim Plot
 Malter Effect

Definitions of Related Terms:

Cold Emission: Another name for field emission.

Electron Field Emission: Another name for field emission.

Fowler-Nordheim Equation and Plot: These describe the field emission, as a function of the applied electric field.

Malter Effect: Field emission induced by a strong field due to surface and internal space charges, causing field emission from the underlying metal.

C. Photoemission:

Common Symbols: A

Common Units: Amp.

Definition: Another subcategory of Electron Emission. This is electron emission due to a photon, of a certain energy, entering the surface of a solid, and imparting its energy to an electron.

In this process the photon's energy will be converted into kinetic energy of the electron; if it is large enough to surmount the surface potential barrier, the electron may escape from the surface.

Related, Derived and/or Associated Terms:Acceptable for Coding:

Current-wavelength characteristic
 Einstein photoelectric law
 Electron photoemission
 Fowler plot
 Photoeffect
 Photoelectric effect
 Photoelectric efficiency
 Photoelectric emission

Photoelectric yield
 Quantum yield
 Relative response
 Specific photosensitivity
 Spectral sensitivity
 Threshold frequency
 X-ray photoemission

Definition of Related Terms:

Current-Wavelength Characteristic: Photoelectric efficiency, considered as a function of photon energy or wavelength.

Einstein Photoelectric Law: When a photon enters a solid its total energy $h\nu$ may be converted into kinetic energy of the electron. The maximum energy with which this electron can leave the surface is

$$T_{\max} = h\nu - E_W,$$

where E_W is the work function of the solid.

Electron Photoemission: Same as photoemission.

Photoeffect: Same as photoemission.

Photoelectric Effect: Same as photoemission.

Photoelectric Efficiency: This is a measure of the efficiency of photoelectric emission, and is defined as the number of emitted electrons per incident photon.

Photoelectric Emission: Same as photoemission.

Photoelectric Yield: Same as photoelectric efficiency.

Quantum Yield: Same as photoelectric efficiency.

Relative Response: Same as photoelectric efficiency.

Specific Photosensitivity: Same as photoelectric efficiency.

Spectral Sensitivity: Same as photoelectric efficiency.

Threshold Frequency: Is the minimum frequency of light that can induce photoelectric emission from a given material.

X-Ray Photoemission: Is photoemission induced by a photon in the x-ray portion of electromagnetic spectrum.

D. Secondary Emission:

Common Symbol: J (Electron Current Density)

Common Units: A/m²

Definition: Another subcategory of electron emission, which is the escape of electrons from the surface as a result of energetic incident electrons hitting the material surface.

Related, Derived and/or Associated Terms:Acceptable for Coding:

Secondary electron emission
 Secondary emission factor
 Secondary emission ratio
 Secondary emission yield
 Secondary gain

Secondary yield
 Secondary yield curve
 Universal yield curve
 Whiddington Law

Definition of Related Terms:

Secondary Electron Emission: Same as secondary emission.

Secondary Emission Factor: Is a measure of the efficiency of secondary emission, and is the average number of secondary electrons emitted per primary incident electron.

Secondary Emission Ratio: Same as secondary emission factor.

Secondary Emission Yield: Same as secondary emission factor.

Secondary Gain: Same as secondary emission factor.

Secondary Yield: Same as secondary emission factor.

Secondary Yield Curve: Curve showing the secondary yield, which gives an idea of the efficiency of secondary emission.

Universal Yield Curve: Curve showing the maximum value of the secondary yield, which varies greatly for some substances such as insulators where a strong field may appear due to surface and internal space charges.

Whiddington Law: Shows the amount of energy loss suffered by a primary electron, upon impinging on a surface, per unit penetration length inside a solid.

Remarks:

When electron emission of a thin layer of one material on another material is reported, system class material directory entries are avoided. Instead, code for physical state thin film, T, for the top material and solid, S, for the bottom material.

MAGNETOELECTRIC PROPERTIES (GP)

Common Symbols: See below

Common Units: See below

Definition: Magnetolectric or galvanomagnetic effects are effects observed when a material carrying an electric current is subjected to a magnetic field.

The best known such effects are the Ettinghausen Effect, the Nernst Effect, magnetoresistance, and the Hall Effect, which was considered separately earlier under Hall Coefficient.

A. Ettinghausen Effect:

Common Symbols: A_E , P

Common Units: deg K - m³/A/Weber

Definition: When a magnetic field is applied perpendicular to an electric current, there results a temperature gradient in a direction perpendicular to both the magnetic field and current.

B. Magnetoresistance:

Common Symbols: $\Delta\rho/\rho$

Common Units: None (dimensionless)

Definition: This is the change in the electrical resistivity of a material when subjected to a magnetic field. The effect is seen for both longitudinal and transverse fields.

At low temperatures, the effect is large and may be strongly affected by impurities.

C. Nernst Effect:

Common Symbols: A_N

Common Units: K - meter/Amp.-Weber²

Definition: This effect is observed when a material is placed in a transverse magnetic field. It is the change in the temperature (thermal) gradient, in the direction of an electric current, when a transverse magnetic field is applied. It differs from the similar Ettinghausen Effect in that here the temperature gradient is longitudinal, rather than transverse.

D. Shubnikov-de Haas Effect:

Common Symbols: Frequently measured as oscillation in the magnitude of the magnetoresistance, dR/dH , with the field or as variation of the period of oscillation with the field.

Common Units: None

Definition: This is the oscillatory dependence of the electrical conductivity of several metals and semi-metals on the magnetic field.

Related, Derived and/or Associated Terms:

Acceptable for Coding:

Ettinghausen Coefficient
Gauss Effect
Magnetoconductivity
Nernst Coefficient

Definitions of Related Terms:

Ettinghausen Coefficient: Shows the extent of this galvanomagnetic effect. It depends on the nature of carrier scattering mechanism, and energy of free carriers.

Gauss Effect: Same as magnetoresistance, but specifically for longitudinal fields.

Magnetoconductivity: Same as magnetoresistivity, but expressed in terms of conductivity.

Nernst Coefficient: A measure of the Nernst Effect. It depends on the thermal conditions normal to the magnetic field on the electric current, and on the scattering, and energy of free carriers.

LUMINESCENCE PROPERTIES (LP)

Common Symbol: τ (decay constant)

Common Units: sec, cd./°K

Defining Equation: $I = I_0 \exp(-t/\tau)$

Definition: Luminescence is light emission that cannot be attributed merely to the temperature of the emitting body.

Luminescence is classified according to the various ways used to cause excitation of atoms or molecules, thus:

- A. Cathodoluminescence: Excitation by fast electrons.
- B. Electroluminescence: Excitation by strong alternating electric fields.
- C. Mechanical Luminescence: Excitation by mechanical impact.
- D. Photoluminescence: Excitation by light, uv, x-ray, etc.
- E. Thermoluminescence: Excitation by heat.

Related, Derived and/or Associated Terms:

Acceptable for coding:

Activator atoms
Cathodoluminescence
Destriau Effect
Electroluminescence
Emission Spectra
Fluorescence
Gudden-Pohl Effect
Intrinsic Electroluminescence
Luminescence Decay Time
Luminescence Glow Curve
Luminescence Recombination
Luminescent Efficiency
Mechanical Luminescence

Phosphorescence
Photoluminescence
Photon Cathodoluminescence
Photon Electroluminescence
Photon Mechanical Luminescence
Photon Photoluminescence
Photon Thermoluminescence
Recombination Radiation
Spontaneous Emission
Stimulated Emission
Stokes Shift
Thermoluminescence

Not Acceptable for Coding:

Chemiluminescence

Definition of Related Terms:

Activator Atoms: Are atoms present in small concentrations in the host lattice, which make luminescence possible.

Cathodoluminescence: Is the luminescence which occurs as a result of excitation of atoms or molecules in a substance by fast electrons.

Destriau Effect: This is photon electroluminescence caused by the action of an alternating current or pulsing electric field on a suspension of luminescent phosphates in a transparent dielectric. This effect is also known as Intrinsic Electroluminescence.

Electroluminescence: Luminescence produced by an alternating current or a pulsing electric field.

Emission Spectrum: Is the spectrum produced by dispersion of light from an excited light source. Excitation here may be thermal, by impacting electrons and ions, or by absorption of photons.

Fluorescence: Luminescence with a temperature-independent decay time of the order of the natural lifetime for allowed radiative transitions in atoms (about 10^{-8} sec.). It gives no noticeable afterglow, in contrast to phosphorescence.

Gudden-Pohl Effect: When an electric field is applied transiently during the afterglow (phosphorescence) of a zinc phosphor, a flash of light is observed as the field is turned off and on. This is the Gudden-Pohl Effect.

Intrinsic Luminescence: Same as Destriau Effect, called thus because luminescence is obtained by means of the electric field alone, with no previous excitation.

Luminescence Decay Time: Is the lifetime or duration of luminescence.

Luminescence Glow Curve: Is the curve showing the light intensity as a function of temperature.

Luminescence Recombination: Is the recombination of holes and electrons, resulting in luminescence.

Luminescent Efficiency: Is the ratio of the probability of decay of crystal excitation by photon emission to the sum of the probabilities of photon and phonon decay.

Mechanical Luminescence: Is the emission of a flash of light from a crystal which has been previously excited optically or thermally, produced by tapping the crystal.

Phosphorescence: Luminescence with a decay time discernible to the eye - in contrast to fluorescence. The decay time is typically temperature dependent.

Photoluminescence: Is the emission of light, where the excitation agent is light - visible, uv or x-ray.

Recombination Radiation: At a p-n junction, electrons from the n-region penetrate the barrier into the p-region and the holes from the p-region move into the n-region. In the new region, these minority carriers recombine with majority carriers, with the emission of light.

Spontaneous Emission: Emission of radiation by an excited system, independently of any de-exciting field. To be contrasted with Stimulated Emission.

Stimulated Emission: Emission of radiation by an excited system, produced by the presence of an electromagnetic field with the same frequency as the emitted radiation.

Thermoluminescence: Is light emission due to the release, by thermal means, of energy stored in a crystal. It is observed as the temperature of the crystal is gradually increased.

MAGNETOMECHANICAL PROPERTIES (MP)

Common Symbols: See below

Common Units: See below

Defining Equations: $\mu_k = f(k, \alpha)$

$\mu_{me} = f(\lambda, \sigma, \alpha)$

$\mu_{mag} = f(N, M)$

Definition: These are a group of properties, involving mechanical changes induced in a material, by application of a magnetic field on it.

Usually, dimensional changes resulting from the magnetization of single crystals are different in different directions - expansion, for instance, in one direction, and contraction in another.

Three forms of energy are involved in these effects.

A. Magneto-Crystalline Anisotropy Energy:

Common Symbols: μ_k, f_k

Common Units: erg/cm³, erg/m³

Definition: Polarization of a magnetic material by a uniform external field involves a change in the free energy that depends on the direction as well as the magnitude of the applied magnetic field, because of the anisotropy of the material. This energy is called the magneto-crystalline anisotropy energy. It can be studied by measuring the torque exerted by the field on the crystal as a function of field orientation.

B. Magneto-Elastic Energy:

Common Symbols: μ_{me}, f_{me}

Common Units: erg/cm³, erg/m³

Definition: Magnetic materials subjected to magnetic fields experience dimensional changes, in general different in different directions, that depend on the strength and direction of the applied field. The energy associated with these dimensional changes is called the magneto-elastic energy.

C. Magnetic Self-Energy or Demagnetization Energy:

Common Symbols: μ_{mag}, f_{mag}

Common Units: erg/cm³, erg/m³

Definition: When a uniform external field is applied to a magnetic body, the field inside the body can be described as the sum of the external field and a demagnetizing field due to the polarized material itself. In establishing the external field, energy to establish the demagnetization field must be supplied. This energy depends on the form of the piece of material considered, as well as its intrinsic magnetic properties, and must be taken into account in thermodynamic treatments of magnetomechanical effects. It is referred to as the magnetic self-energy or the demagnetization energy.

Related, Derived and/or Associated Terms:

Acceptable for Coding:

| | |
|-----------------------------------|---|
| Anisotropy Constants | Magneto-Elastic Energy |
| Anisotropy Energy | Magneto-Elastic Expansivity |
| Demagnetization | Magnetostriction |
| Demagnetization Energy | Magnetostriction Constant |
| Demagnetizing Coefficient | Magnetostrictive Coefficient |
| Guillemin Effect | Magnetostrictive Energy |
| Magnetic Self-Energy | Saturation Magnetostriction Coefficient |
| Magneto-Crystalline Energy | Villari Effect |
| Magnetoelastic Constants | Wiedmann Effect |
| Magnetoelastic Coupling Constants | |

Not Acceptable for Coding:

| | |
|-------------------|--------|
| Elastic Constants | Strain |
| Magnetization | Stress |

Definition of Related Terms:

Anisotropy Constants: These are the constants in the equation for the magneto-crystalline anisotropy energy of a crystal.

Guillemin Effect: Is a magnetostrictive effect, whereby a bar of ferromagnetic material, elastically or permanently bent, tends to straighten upon magnetization.

Magnetoelastic Constants: These appear in the equation for the magneto-elastic energy.

Magnetoelastic Coupling Constants: The sum of the elastic energy density and the magnetic anisotropy density contains magnetoelastic coupling terms - terms that depend both on the applied field and the elastic strains in the body. The presence of these terms is responsible for magnetostrictive effects. The constants in these terms are known as magnetoelastic coupling constants.

Magnetostriction: This is the dimensional change occurring in a material during magnetization.

Magnetostrictive Energy: This is the amount of mechanical work required to induce a specific magnetostriction.

Saturation Magnetostriction Coefficient: Is the fractional change in the length of the sample, when magnetized from the ideal demagnetized state to saturation.

Villari Effect: The magnetization of a material, in the presence of a field, is altered upon the application of external stress. In certain materials, under conditions of high field strength, the magnetostriction effect changes sign, i. e., the direction of dimensional change reverses.

Weidmann Effect: This is the twist produced in a wire, placed in a longitudinal magnetic field, when a current flows through the wire. The magnetic material expands or contracts parallel to the resultant lines of force, and hence the twists.

The inverse Weidmann effect is the axial magnetization of a current-carrying wire when twisted.

PHOTOELECTRONIC PROPERTIES (PP)

Common Symbols: See below

Common Unit: See below

Definition: This group of properties comprises those phenomena in which light incident on a crystal results in the generation of a potential across the crystal. Included here are the Dember Effect, photoconductivity, photomagnetic effect, photopiezoelectric effect and the photovoltaic effect.

A. Dember Effect:

Common Symbols: V_D

Common Units: Volts

Definition: This effect, sometimes called the photodiffusion effect, is the appearance of a potential difference between unequally illuminated regions of a semiconductor. The illumination generates hole-electron pairs, and their varying concentration and unequal diffusion creates an overall charge imbalance, thus giving rise to a potential difference.

B. Photoconductivity:

Common Symbols: $\Delta\sigma/\sigma$

Common Units: None (Dimensionless)

Definition: This is the fractional change in the electrical conductivity of a semiconductor or insulator, per unit incident radiant energy or per photon, when the material is irradiated with light.

By various mechanisms, electrons in the highest occupied bands are excited and elevated to a higher unoccupied band above, known as the conduction band, where they participate in electronic conduction.

C. Photomagnetic Effect:

Common Symbols: P. M. E., P. E. M.

Common Units: None

Definition: This effect is noted when a photoconductive material is placed in a magnetic field, and illuminated in a direction perpendicular to the field. It is found that a voltage appears across the face of the material in a direction perpendicular

to both the magnetic field and the beam of light. This effect is also called the photoelectromagnetic effect, the magnetophotovoltaic effect, the P.E.M., or the P.M.E. effect.

As yet a P.E.M. coefficient hasn't been defined. The effect is used in photoconductive measurements to determine very short carrier lifetimes.

D. Photopiezoelectric Effect:

Common Symbols: V

Common Units: Volts

Definition: This is the effect of inhomogeneous strains on illuminated semiconductors, whereby a potential difference is generated. The change in strain from one region to another leads to variation in the energy gap (which is strain dependent), which in turn gives rise to the photopotential.

E. Photovoltaic Effect:

Common Symbols: V_L

Common Units: Volts

Definition: This is the process by which an electric potential (photovoltage) is generated at the junction of two dissimilar materials by an incident photon flux. This measured photovoltage is a function of the exciting light intensity.

Related, Derived and/or Associated Terms:

Acceptable for Coding:

| | |
|----------------------------|-------------------------------------|
| Dark Conductivity | Photocurrent |
| Dember Potential | Photodielectric Effect |
| Internal Photoeffect | Photodiffusion |
| Magnetophotovoltaic Effect | Photoelectromagnetic Effect |
| Optical Conductivity | Photoelectromotive Force (e. m. f.) |
| Optoelectric Effect | P. M. E. Effect |
| P. E. M. Effect | Radioelectric Effect |
| Photocapacitance | |

Definition of Related Terms:

Dark Conductivity: Is the conductivity at the dark region of a material, induced by illumination of another part of it.

Dember Potential: Is the voltage generated in connection with the Dember Effect.

Magnetophotovoltaic Effect: Another name for photomagnetic effect.

Optical Conductivity: Is the electrical conductivity of a material at very high frequencies.

P. E. M. and P. M. E. Effect: Are the abbreviations of photoelectromagnetic and photomagnetolectric effects, respectively - both of which are the same as photomagnetic effect.

Photocurrent: Is the current flow generated during the photovoltaic effect.

Photodiffusion: Another name for the Dember Effect.

Photoelectromagnetic Effect: Same as the photomagnetic effect.

Photoelectromotive Force (Photo-e. m. f.): Is the voltage or potential difference arising during the photovoltaic effect.

THERMOELECTRIC PROPERTIES (TP)

Common Symbols: See below

Common Units: V - °K, Volts, V/°K, μ V

Defining Equations: $E' = \sigma(dT/d\ell)$

$$\xi = \int_{\tau_1}^{\tau_2} \sigma dT$$

$$\xi_{AB} = \xi_{AC} - \xi_{BC}$$

Definition: There are properties related to phenomena exhibited by conductors made up of two or more different materials in contact with each other, in the presence of both electric fields and temperature gradients.

There are three main effects here: The Peltier Effect, the Seebeck Effect, and the Thomson Effect.

A. Peltier Effect:

Common Symbols: π

Common Units: Volts

Definition: The Peltier e. m. f. arises when two dissimilar conductors at the same temperature are brought into contact, and a diffusion of electrons takes place from one conductor to the other - due to the difference in the work functions of the two conductors. This diffusion or flow of electrons will set up a potential difference across the two conductors, which increases until there is no more electron flow, and equilibrium is attained.

This e. m. f. is dependent on the temperature of the junction as well as on the metals involved.

B. Seebeck Effect:

Common Symbols: S, ϵ

Common Units: Volts/Degree

Definition: The Seebeck e. m. f. that arises in a closed circuit formed by two dissimilar metals, with two junctions at different temperatures.

This is actually the sum of the e. m. f. 's due to the Thomson and Peltier Effects in the circuit, and depends only on the temperatures of the junctions.

In tables relating to thermoelectricity it is customary to provide tables of the Thermoelectric Power of a given metal with respect to some reference metal, such as lead or platinum. If $\xi_{AC}(T)$ denotes the Seebeck e. m. f. in a circuit made up of metal A and reference metal C, when one junction is at temperature T and the other is at reference temperature T_R , the thermoelectric power ϵ_A of metal A at temperature T (with respect to the specified reference metal) can be defined as

$$\epsilon_A(T) = \frac{d \xi_{AC}(T)}{dT}.$$

$\epsilon_A(T)$ is independent of T_0 . The Seebeck e. m. f. in a circuit consisting metals A and B with junctions at temperatures T_1 and T_2 can be determined from $\epsilon_A(T)$ and $\epsilon_B(T)$ as

$$\xi = \int_{T_1}^{T_2} (\epsilon_A - \epsilon_B) dT.$$

C. Thomson Effect:

Common Symbols: σ, ϵ

Common Units: Volts-Degree

Definition: This is the e. m. f. arising from the temperature gradient in the same circuit element. This temperature gradient in a metal, creates a gradient of energy of the electrons, and hence mobility differences. This subsequently will give rise to a flow of electrons, until a potential difference or an electric field is set up which is just sufficient to counter-balance this flow.

Related, Derived and/or Associated Terms:

Acceptable for Coding:

Figure of Merit
Peltier Coefficient
Peltier Effect
Peltier e. m. f.
Peltier Heat
Seebeck Coefficient
Seebeck Effect
Seebeck e. m. f.

Seebeck Potential
Thermoelectric Coefficients
Thermoelectric Effectiveness
Thermoelectric Figure of Merit ($^{\circ}\text{K}^{-1}$)
Thermoelectric Power
Thomson Coefficient
Thomson Effect
Thomson e. m. f.

Definition of Related Terms:

Figure of Merit: It is a parameter defined for thermoelectric materials, relating the thermoelectric power, electrical conductivity and the thermal conductivity of the material, such that the higher the value of this parameter is, the better is the substance as a thermoelectric material.

Peltier Coefficient: The Peltier Coefficient π_{AB} of a junction of metals A and B at temperature T is defined as the amount of heat absorbed per unit charge flowing from A to B. It is related to the Thermoelectric Power of the metals at the same T by

$$\pi_{AB} = T(\epsilon_A - \epsilon_B).$$

Peltier Heat: When a current flows through a junction between two metals, there is a reversible flow of heat into or out of the junction that is proportional to the charge transferred. This is called the Peltier Heat.

Thermoelectric Coefficients: Are any of the constants characterizing a thermoelectric material, e.g., Thomson, Peltier, or Seebeck Coefficient.

Thermoelectric Figure of Merit: Same as figure of merit.

Thermoelectric Power: See under Seebeck Effect, page 133.

Thomson Coefficient: The Thomson Coefficient σ_A is defined by the equation

$$\Delta Q = I \sigma_A \Delta T,$$

where ΔQ is the Thomson Heat absorbed per second in an element of wire of metal A due to flow of current I through temperature difference ΔT , in the direction of increasing T. Thermodynamic arguments show that

$$\sigma_A - \sigma_B = -T \frac{d}{dT} (\epsilon_A - \epsilon_B).$$

Thomson Heat: When a current flows through a wire in which there is a temperature gradient, there will be a reversible emission or absorption of heat proportional to the change transferred and to the temperature gradient. This is the Thomson Heat.

Remarks:

For thermoelectric properties, system class material directory entries are avoided. Instead separate code lines are written for the two materials in contact. When one of the materials is a reference, such as lead or platinum, it is not necessary to write a code line for this material.

PIEZOELECTRIC PROPERTIES (ZP)

Common Symbols: d_{kl}^i , γ , γ' , γ'' , k

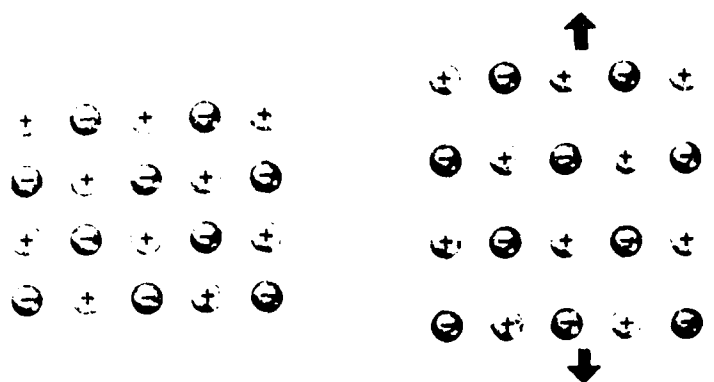
Common Units: γ (Coulombs/cm² deg C), other constants dimensionless

Defining Equation: $d_{kl}^i = \Delta P_i / \Delta \sigma_{kl}$

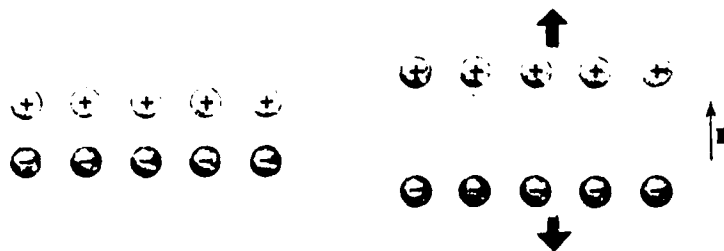
Definition: These are effects arising from the interaction of strains and electric polarization in crystals.

For example, application of a mechanical stress or strain to a crystal may induce an electric polarization of it; this is the piezoelectric effect.

If an electric field is applied to such a crystal, the crystal changes its shape; this is the inverse piezoelectric effect.



(a) Tensile strain of ionic crystal with center of symmetry (any lattice site). No induced dipole moment



(b) Tensile strain of ionic crystal with no symmetry center, showing strain induced dipole moment

Figure II-14. Piezoelectricity and Crystal Symmetry. In Crystals Lacking a Center of Symmetry an Elastic Strain Induces a Dipole Moment. (From Rose, R. M., Shepard, L. A., Wulff, J., The Structure and Properties of Materials, Vol. IV: Electronic Properties.)

Related, Derived and/or Associated Terms:Acceptable for Coding:

| | |
|-----------------------------------|-------------------------------------|
| Coupling Coefficients | Piezoelectricity |
| Direct Piezoelectric Effect | Primary Pyroelectric Coefficient |
| Electromechanical Coupling Factor | Pyroelectric Effect |
| Electrostriction | Pyroelectricity |
| Inverse Piezoelectric Effect | Secondary Pyroelectric Polarization |
| Piezoelectric Coefficient | Tertiary Pyroelectric Effect |
| Piezoelectric Constants | Total Pyroelectric Coefficient |
| Piezoelectric Effect | |

Not Acceptable for Coding:

| | |
|---------------------|--------|
| Elastic Constants | Strain |
| Mechanical Q Factor | Stress |
| Polarization | |

Definition of Related Terms:

Coupling Coefficients: These are numerical values between 0 and 1, characterizing the degree of coupling between two mechanically vibrating systems. Maximum coupling is 1, and no coupling is zero.

Direct Piezoelectric Effect: Defined in the main definition.

Electrostriction EME: This is the change in dimensions of a dielectric, due to an applied field.

Inverse Piezoelectric Effect: Defined in the main definition.

Piezoelectric Coefficients: Are ratios of changes of the electrical polarization to changes of elastic stresses or strains - hence piezoelectric stress coefficients and piezoelectric strain coefficients.

Piezoelectric Constants: Same as piezoelectric coefficients.

Piezoelectric Effect: Defined in the main definition.

Piezoelectricity: Is the same as piezoelectric effect.

Primary Pyroelectric Coefficient: Change in temperature of a completely clamped crystal (that is, one held at constant dimensions) will cause a change in the polarization of pyroelectric material. The primary pyroelectric coefficient is the temperature derivative of this polarization.

Pyroelectricity: Crystals exhibiting the pyroelectric effect are spontaneously polarized at any temperature, but due to atmospheric leakage, the surface charge is quickly neutralized. The polarization of the crystal becomes apparent during the transient period following a temperature change.

Pyroelectric Effect: Is the spontaneous polarization of a substance which becomes apparent when it undergoes a change in temperature. Here there is a net polarization.

Secondary Pyroelectric Polarization: Change in the temperature of a free pyroelectric crystal will cause a change in its dimensions, which will in turn produce a change in its polarization that is superposed on the change due to the change in temperature alone. This is referred to as secondary pyroelectricity, and its temperature derivative is the secondary pyroelectric coefficient.

Total Pyroelectric Coefficient: This is the ratio of the change of the electrical polarization to the change of the temperature, and is actually the sum of the primary and secondary coefficients.

APPENDIX III

REFERENCE LITERATURE FOR SUBSTANCE IDENTIFICATION

It is often necessary for the coder to consult handbooks and dictionaries to determine the exact name, formula, or composition for a given substance. The following list of selected references provides useful sources of substance identification:

1. "Aluminum Standards and Data," The Aluminum Association.
2. "Chemical Abstracts--Subject Index and Formula Index."
3. "Chemical Synonyms and Trade Names: A Dictionary and Commercial Handbook," W. Gardner and E. I. Cooke.
4. "The Condensed Chemical Dictionary," A. and E. Rose.
5. "Designations of Alloys for Aircraft and Missiles" (DMIC Memorandum 177).
6. "Engineering Alloys," N. E. Woldman.
7. "Glossary of Geology," M. Gary, R. McAfee, Jr., C. L. Wolf.
8. "Handbook of Chemistry and Physics."
9. "Handbook of Designations and Specifications for Soviet Nonmetallic Polymeric Materials," Volumes 1-6.
10. "Handbook of Material Trade Names," O. T. Zimmerman and I. Lavine.
11. "Handbook of Soviet Alloy Compositions."
12. "Material Properties Handbook: Volume I--Aluminum Alloys, Volume II--Steels, Volume III--Magnesium, Nickel and Titanium Alloys, Volume IV--Heat Resisting Alloys."
13. "The Mechanical and Physical Properties of the British Standard EN Steels: Volume 1--EN1-EN20, Volume 2--EN21-EN39," Woolman, J. and Mottram, R. A.
14. "The Merck Index of Chemicals and Drugs."
15. "Metal Industry: Handbook and Directory."
16. "Metallic Materials Specification Handbook," R. B. Ross.
17. "Metal Selector."
18. "Metals Handbook: Volume 1--Properties and Selection of Metals."
19. "Modern Plastics Encyclopedia."
20. "Pocketbook of AISI Standard Steels," American Iron and Steel Institute.
21. "The Ring Index," A. M. Patterson, L. T. Capell, and D. F. Walker.
22. "Stahl-Eisen-Liste," H. Schmitz.
23. "Standards Handbook," Copper Development Association, Inc.
24. "Synthetic Organic Chemical Manufacturers Association Handbook: Commercial Organic Chemical Names."
25. "Unified Numbering System for Metals and Alloys."
26. "Wrought Steels-British Standard 970:1955," British Standards Institution.

APPENDIX IV

THE SUPPLEMENTARY INDEX: DICTIONARY OF SYNONYMS AND
TRADE NAMES WITH A LISTING OF CROSS REFERENCES

This index is an essential tool in the preparation and use of the Retrieval Guide. (Internally, it is referred to as the Synonyms Index.) The choice of names for a substance which has several possible synonyms must be consistent. The Synonyms Index provides the correct identification of a substance name as adopted by TEPIAC.

It is pertinent that any newly encountered synonym or trade name be immediately added to the separate index list maintained by the coders. The editor is the only person who makes the actual entries into the Synonyms Index, in order that the synonym list may be fully coordinated with the Directory of Substances.

A sample of the Synonym Index format follows:

| <u>Synonym</u> | <u>Name Used by TEPIAC</u> | <u>Class</u> |
|----------------|----------------------------|--------------|
| Alumina | Aluminum oxide | 102-0002 |
| Alumina | Corundum | 521-0077 |
| Alumina | Porcelain, aluminum oxide | 503-0714 |
| Alumina | Refractory, aluminum oxide | 503-0865 |
| Alumina | Ruby | 521-0191 |
| Alumina | Sapphire | 521-0064 |
| Vinegar acid | Acetic acid | 221-0081 |
| Vinyl chloride | Chloroethylene | 206-0060 |

APPENDIX V

CLASSIFICATION OF REFRIGERANTS

* Methane Derivatives

| | | | | | | | | | |
|----|---------------------------------|----|---------------------|----|---------------------------------|----|--------------------|----|-----------------|
| 10 | CCl ₄ | 11 | CFCl ₃ | 12 | CF ₂ Cl ₂ | 13 | CF ₃ Cl | 14 | CF ₄ |
| 20 | CHCl ₃ | 21 | CHFCl ₂ | 22 | CHF ₂ Cl | 23 | CHF ₃ | | |
| 30 | CH ₂ Cl ₂ | 31 | CH ₂ FCl | 32 | CH ₂ F ₂ | | | | |
| 40 | CH ₃ Cl | 41 | CH ₃ F | | | | | | |
| 50 | CH ₄ | | | | | | | | |

† Ethane Derivatives

| | | | | | | | | | | | | | |
|-----|---|-----|--|-----|--|-----|---|-----|---|-----|----------------------------------|-----|-------------------------------|
| 110 | C ₂ Cl ₆ | 111 | C ₂ FCl ₅ | 112 | C ₂ F ₂ Cl ₄ | 113 | C ₂ F ₃ Cl ₃ | 114 | C ₂ F ₄ Cl ₂ | 115 | C ₂ F ₅ Cl | 116 | C ₂ F ₆ |
| 120 | C ₂ HCl ₅ | 121 | C ₂ HFCl ₄ | 122 | C ₂ HFCl ₃ | 123 | C ₂ HF ₂ Cl | 124 | C ₂ HF ₃ Cl | 125 | C ₂ HF ₄ | | |
| 130 | C ₂ H ₂ Cl ₄ | 131 | C ₂ H ₂ FCl ₃ | 132 | C ₂ H ₂ F ₂ Cl ₂ | 133 | C ₂ H ₂ F ₃ Cl | 134 | C ₂ H ₂ F ₄ | | | | |
| 140 | C ₂ H ₃ Cl ₃ | 141 | C ₂ H ₃ FCl ₂ | 142 | C ₂ H ₃ F ₂ Cl | 143 | C ₂ H ₃ F ₃ | | | | | | |
| 150 | C ₂ H ₄ Cl ₂ | 151 | C ₂ H ₄ FCl | 152 | C ₂ H ₄ F ₂ | | | | | | | | |
| 160 | C ₂ H ₅ Cl | 161 | C ₂ H ₅ F | | | | | | | | | | |
| 170 | C ₂ H ₆ | | | | | | | | | | | | |

* Copied from: Rombusch, U. K., Kältetechnik, 15, 353, 1963.

†

PROPANE DERIVATIVES

| | | | |
|--------------|-----------------|-----------------|---------------|
| 210 | | 211 | |
| C_3Cl_8 | | C_3FCl_7 | |
| 220 | 221 | 212 | |
| C_3HCl_7 | C_3HFCl_6 | $C_3F_2Cl_6$ | |
| 230 | 231 | 222 | 213 |
| $C_3H_2Cl_6$ | C_3HFCl_5 | $C_3HF_2Cl_5$ | $C_3F_3Cl_5$ |
| 240 | 232 | 223 | 214 |
| $C_3H_3Cl_5$ | $C_3H_2F_2Cl_4$ | $C_3HF_3Cl_4$ | $C_3F_4Cl_4$ |
| 250 | 241 | 233 | 215 |
| $C_3H_4Cl_4$ | $C_3H_3F_2Cl_3$ | $C_3HF_4Cl_3$ | $C_3F_5Cl_3$ |
| 260 | 251 | 242 | 216 |
| $C_3H_5Cl_3$ | $C_3H_4F_2Cl_2$ | $C_3H_3F_3Cl_2$ | $C_2HF_5Cl_2$ |
| 270 | 261 | 243 | 217 |
| $C_3H_6Cl_2$ | $C_3H_4F_2Cl_2$ | $C_3H_3F_4Cl_2$ | $C_3F_6Cl_2$ |
| 280 | 262 | 244 | 218 |
| C_3H_7Cl | $C_3H_5F_2Cl$ | $C_3H_4F_3Cl$ | C_3HF_6Cl |
| 290 | 271 | 245 | 227 |
| C_3H_8 | $C_3H_6F_2$ | $C_3H_5F_3$ | C_3HF_7 |
| | 272 | 254 | 228 |
| | C_3H_7F | $C_3H_4F_4$ | $C_3H_2F_6$ |
| | | 255 | $C_3H_3F_5$ |
| | | 263 | $C_3H_2F_6$ |
| | | 264 | C_3HF_7 |
| | | 265 | C_3F_8 |

Compiled by
P. E. Liley
October 1968

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