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François Cardarelli

Materials Handbook

A Concise Desktop Reference

Second Edition

哈爾濱工業大學出版社
HARBIN INSTITUTE OF TECHNOLOGY PRESS

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本手册提供各种材料的物理和化学性质,是一本简洁的手边工具书。第二版与第一版的差别是扩充了新的家用材料,但重点是每一类常见的工业材料。

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François Cardarelli

Materials Handbook

A Concise Desktop Reference

2nd Edition

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Dedication for the First Edition

The ***Materials Handbook*: *A Concise Desktop Reference*** is dedicated to my father, Antonio, and my mother, Claudine, to my sister, Elsa, and to my spouse Louise Saint-Amour for their love and support. I want also to express my thanks to my two parents and my uncle Consalvo Cardarelli, which in close collaboration have provided valuable financial support when I was a teenager to contribute to my first fully equipped geological and chemical laboratory and to my personal comprehensive scientific library. This was the starting point of my strong and extensive interest in both science and technology, and excessive consumption of scientific and technical literature.

François Cardarelli

Dedication for the Second Edition

The ***Materials Handbook: A Concise Desktop Reference*** is dedicated to my father, Antonio, and my mother, Claudine, to my sister, Elsa, and to my wife Elizabeth I.R. Cardarelli for their love and support. I want also to express my thanks to my two parents and my uncle Consalvo Cardarelli, which in close collaboration have provided valuable financial support when I was a teenager to contribute to my first fully equipped geological and chemical laboratory and to my personal comprehensive scientific library. This was the starting point of my strong and extensive interest in both science and technology, and excessive consumption of scientific and technical literature.

François Cardarelli

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Mr. Anthony Doyle (senior engineering editor), Mr. Oliver Jackson (associate engineering editor), and Mr. Nicolas Wilson (editorial coordinator) are gratefully acknowledged for their valued assistance, patience, and advice.

Units Policy

In this book the only units of measure used for describing physical quantities and properties of materials are those recommended by the *Système International d'Unités* (SI). For accurate conversion factors between these units and the other non-SI units (e.g., cgs, fps, Imperial, and US customary), please refer to the reference book by the same author:

Cardarelli, F. (2005) *Encyclopaedia of Scientific Units, Weights, and Measures. Their SI Equivalences and Origins.* Springer, London New York. ISBN 978-1-85233-682-1.

Author Biography

Dr. François Cardarelli (Ph.D.)
Born in Paris (France) February 17, 1966
Canadian citizen

Academic Background

- Ph.D., chemical engineering (Université Paul Sabatier, Toulouse, France, 1996)
- Postgraduate degree (DEA) in electrochemistry (Université Pierre et Marie Curie, Paris, 1992)
- M.Sc. (Maîtrise), physical chemistry (Université Pierre et Marie Curie, Paris, 1991)
- B.Sc. (Licence), physical chemistry (Université Pierre et Marie Curie, Paris, 1990)
- DEST credits in nuclear sciences and technologies (Conservatoire National des Arts et Métiers, Paris, 1988)

- Associate degree (DEUG B) in geophysics and geology (Université Pierre et Marie Curie, Paris, 1987)
- Baccalaureate C (mathematics, physics, and chemistry) (CNED, Versailles, France, 1985)

Fields of Professional Activity

The author has worked in the following areas (in chronological order) since 1990.

(1) Research scientist at the Laboratory of Electrochemistry (Université Pierre & Marie Curie, Paris, France) for the development of a nuclear detector device for electrochemical experiments involving radiolabeled compounds;

(2) research scientist at the Institute of Marine Biogeochemistry (CNRS & École Normale Supérieure, Paris, France) for the environmental monitoring of heavy-metal pollution by electroanalytical techniques;

(3) research scientist for the preparation by electrochemistry in molten salts of tantalum protective thin coatings for the chemical-process industries (sponsored by Electricité de France);

(4) research scientist for the preparation and characterization of iridium-based industrial electrodes for oxygen evolution in acidic media at the Laboratory of Electrochemical Engineering (Université Paul Sabatier, Toulouse, France);

(5) registered consultant in chemical and electrochemical engineering (Toulouse, France);

(6) battery product leader in the technology department of ARGOTECH Productions, Boucherville (Québec), Canada, in charge of electric-vehicle, stationary, and oil-drilling applications of lithium polymer batteries;

(7) materials expert and industrial electrochemist in the lithium department of ARGOTECH Productions, involved in both the metallurgy and processing of lithium metal anodes and the recycling of spent lithium polymer batteries;

(8) materials expert and industrial electrochemist in the technology department of AVESTOR, Boucherville (Quebec), Canada, in charge of all strategic raw materials entering into the fabrication of lithium polymer batteries, as well as being in charge of the recycling process of spent lithium batteries;

(9) principal chemist, materials, in the technology department of RIO TINTO Iron and Titanium, Sorel–Tracy (Québec), Canada working on the electrowinning of titanium metal from titania-rich slags and on other novel electrochemical processes;

(10) principal electrochemist at Materials and Electrochemical Research (MER) Corp., Tuscon (Arizona, USA) working on the electrowinning of titanium metal powder from composite anodes and other materials related projects.

Introduction

Despite the wide availability of several comprehensive series in materials sciences and metallurgy, it is difficult to find grouped properties either on metals and alloys, traditional and advanced ceramics, refractories, polymers and elastomers, composites, minerals and rocks, soils, woods, cement, and building materials in a single-volume source book.

Actually, the purpose of this practical and concise reference book is to provide key scientific and technical materials properties and data to materials scientists, metallurgists, engineers, chemists, and physicists as well as to professors, technicians, and students working in a broad range of scientific and technical fields.

The classes of materials described in this handbook are as follows:

(i) metals and their alloys;
(ii) semiconductors;
(iii) superconductors;
(iv) magnetic materials;
(v) dielectrics and insulators;
(vi) miscellaneous electrical materials (e.g., resistors, thermocouples, and industrial electrode materials);
(vii) ceramics, refractories, and glasses;
(viii) polymers and elastomers;
(ix) minerals, ores, and gemstones;
(x) rocks and meteorites;
(xi) soils and fertilizers;
(xii) timbers and woods;
(xiii) cement and concrete;
(xiv) building materials;
(xv) fuels, propellants, and explosives;

(xvi) composites;
(xvii) gases;
(xviii) liquids.

Particular emphasis is placed on the properties of the most common industrial materials in each class. The physical and chemical properties usually listed for each material are as follows:

(i) physical (e.g., density, viscosity, surface tension);
(ii) mechanical (e.g., elastic moduli, Poisson's ratio, yield and tensile strength, hardness, fracture toughness);
(iii) thermal (e.g., melting and boiling point, thermal conductivity, specific heat capacity, coefficients of thermal expansion, spectral emissivities);
(iv) electrical (e.g., resistivity, relative permittivity, loss tangent factor);
(v) magnetic (e.g., magnetization, permeability, retentivity, coercivity, Hall constant);
(vi) optical (e.g., refractive indices, reflective index, dispersion, transmittance);
(vii) electrochemical (e.g., Nernst standard electrode potential, Tafel slopes, specific capacity, overpotential);
(viii) miscellaneous (e.g., relative abundances, electron work function, thermal neutron cross section, Richardson constant, activity, corrosion rate, flammability limits).

Finally, detailed appendices provide additional information (e.g., properties of the pure chemical elements, thermochemical data, crystallographic calculations, radioactivity calculations, prices of metals, industrial minerals and commodities), and an extensive bibliography completes this comprehensive guide. The comprehensive index and handy format of the book enable the reader to locate and extract the relevant information quickly and easily. Charts and tables are all referenced, and tabs are used to denote the different sections of the book. It must be emphasized that the information presented here is taken from several scientific and technical sources and has been meticulously checked and every care has been taken to select the most reliable data.

Contents

5 Semiconductors

5.1 Band Theory of Bonding in Crystalline Solids

The theory of chemical bonding in crystalline solids such as pure metals and alloys, insulators, and semiconductor materials may be well understood by an expansion of the ***linear combination of atomic orbitals***. Actually, the atomic orbitals (AO) of two atoms could be combined together to form bonding and antibonding molecular orbitals (MO) symbolized by σ and σ^*, respectively. In the case of three neighboring atoms, this creates a string of atoms with bonding that connects all three. Hence, there appear a bonding orbital, an antibonding orbital, and a new orbital called a nonbonding orbital. Essentially a nonbonding orbital is an orbital that neither increases nor decreases the net bonding energy in the molecule. The important feature here is that three atomic orbitals must produce three molecular orbitals. Hence, the total number of orbitals must remain constant. If we apply this concept by considering combinations of four atoms, it will give four molecular orbitals, two bonding and two antibonding. Notice that the two bonding and two antibonding orbitals do not have exactly the same energy. The lower bonding orbital is slightly more bonding than the other, and, similarly, one antibonding orbital is slightly more antibonding than the other. As a general rule, if we consider a large number of atoms, N, where N could have an order of magnitude similar to that of Avogadro's number, it will lead to the combination of a large number of bonding and antibonding orbitals. These orbitals will be so close together in energy that they will begin to overlap, creating a definite band of bonding (i.e., highest occupied (HO) energy band or ***valence band***) and a band of antibonding orbitals (i.e., lowest unoccupied (LU) or ***conduction band***). The empty energy region between the valence and conduction bands is called the ***energy-band gap***. These definitions arise because electrons that enter the antibonding band are free to move about the crystal under an electric field (i.e., electrical conduction). It is the existence of valence and conduction bands that explains the electrical and optical properties of crystalline solids. The ***Fermi level***, with an energy E_F, is a level whose probability of being occupied by an electron is 1/2. The Fermi level is the highest occupied state at absolute zero (i.e., –273.15°C).

5.2 Electrical Classification of Solids

Atoms of a metal have many unoccupied levels with similar energies. A large number of mobile electric charge carriers are able to move across the material when an electrical potential difference (i.e., voltage) is applied. In a semiconductor or insulator, the valence band is completely filled with electrons in bonding states, so that conduction cannot occur. There are no vacant levels of similar energy on neighboring atoms. At absolute zero, its antibonding states (i.e., the conduction band) are completely empty, with no electrons there able to conduct electricity. For this reason, insulators cannot conduct. In the case of semiconductors, as the temperature increases, electrons in the valence band acquire, due to the Brownian thermal motion, sufficient kinetic energy to be promoted across the energy-band gap into the conduction band. When this occurs, these promoted electrons can move and conduct electricity. Therefore, the narrower the energy-band gap, the easier it is for electrons to jump to the conduction band. Hence, according to the theory of bands, in crystalline solids, it is possible to classify solids into three distinct categories of materials (Figure 5.1):

(i) Solids that exhibit a large energy-band gap above 3.0 eV (i.e., 290 kJ/mol) are called electric ***insulators.***

(ii) Solids with an energy-band gap between 0.01 and 3.0 eV (i.e., 0.965 to 290 kJ/mol) are said to be ***semiconductors.***

(iii) Solids with effectively no gap (i.e., zero gap) or a gap below 0.001 eV are called ***conductors*** (i.e., pure metals and most alloys).

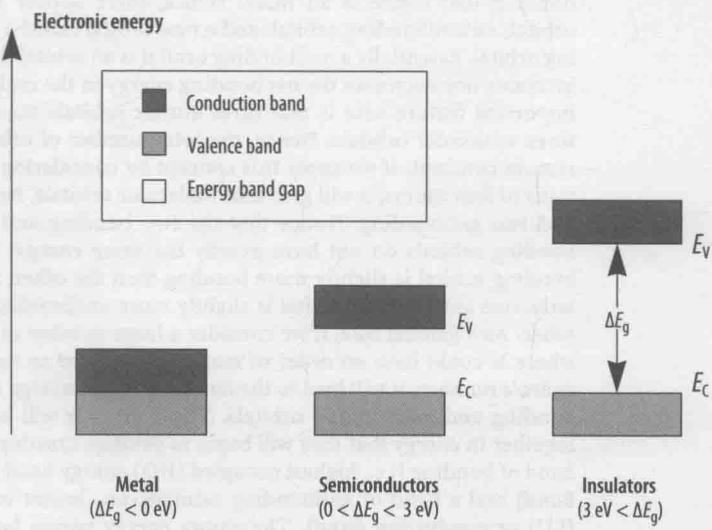

Figure 5.1. Electrical classification of solids

For instance, the most common orders of magnitude for energy-band gaps are 5.3 eV (511 kJ/mol) for diamond-type Ia, showing its excellent electric insulating properties, and 1.04 eV (i.e., 100 kJ/mol) for pure silicon (Si) monocrystal used as semiconductors and 0.69 eV (i.e., 67 kJ/mol) for pure germanium (Ge) crystals. The first two examples are both intrinsic semiconductors. Moreover, electrical conductivity of materials is strongly temperature dependent. In fact, as the temperature increases, the conductivity of metals decreases, while the electrical conductivity of pure semiconductors and insulators increases.

A general trend of the properties of chemical elements in the periodic table is that the ***metallic character*** of the chemical elements increases when moving from the upper right to the left and bottom of the periodic chart. Therefore, it would be expected that the most metallic elements would be found in the lower left corner of the table and the least metallic in the upper right. However, there is a gradual transition of properties from metallic to nonmetallic elements when moving to the top right of the periodic table. This rule of the thumb can be useful to compare quickly the electrical properties of two elements. The two intermediate chemical elements of group IVA(14) of the periodic chart exhibit properties that are intermediate between metallic (e.g., Sn and Pb) and nonmetallic (e.g., C and diamond) and hence can be characterized as semiconductors (e.g., Si and Ge). Actually these elements exhibit the diamond crystal structure, and both pure silicon and germanium behave as perfect insulators at absolute zero temperature (–273.15°C), but at moderate temperatures their resistance to the flow of electricity decreases measurably. Since they never become good conductors, they are classified as electrical semiconductors (sometimes called *semimetals* or *metalloids* in old textbooks).

5.3 Semiconductor Classes

Semiconductors are defined as crystalline or amorphous solid materials that carry an electric current by electromigration of both electrons and holes and have an energy-band gap of between 0.0 and 3.0 eV. The main characteristic of semiconductors, by contrast with metals, is the exponential rise of the electric conductivity with the increase of temperature. Moreover, another important property of semiconductors is their ability to decrease their electrical resistivity at a given temperature by ***doping***, i.e., introducing a definite amount of traces of electrically active impurities. As a general rule, semiconductors have electrical resistivities with values between 10 μΩ.cm and 10 MΩ.cm. However, the semiconductors group can also be split into three main groups:

(i) ***intrinsic*** or ***elemental semiconductors***;
(ii) extrinsic ***doped*** or ***type-p semiconductors*** and extrinsic ***doped or type-n semiconductors***;
(iii) ***extrinsic*** or ***compound semiconductors.***

5.3.1 Intrinsic or Elemental Semiconductors

Intrinsic semiconductive materials and intrinsic semiconductors are solids having an energy-band gap of between 0 and 3eV and hence are electrical insulator under normal conditions, but they can become good electrical conductors under certain circumstances such as temperature increase or under electromagnetic irradiation. Intrinsic semiconductors are especially the pure elements of group IVA(14) of Mendeleev's periodic chart., i.e., silicon (Si), germanium (Ge), and alpha-tin (α-Sn), with intentional doping and having a diamond crystal space lattice structure. Owing to their electronic configuration, the atoms in this class have exactly enough outer-shell electrons ns^2np^2 to fill the valence or bonding band while the