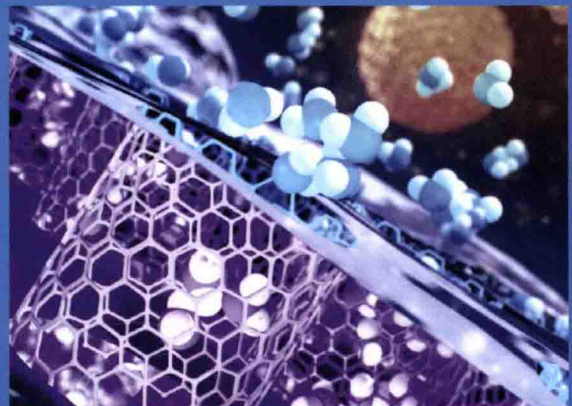
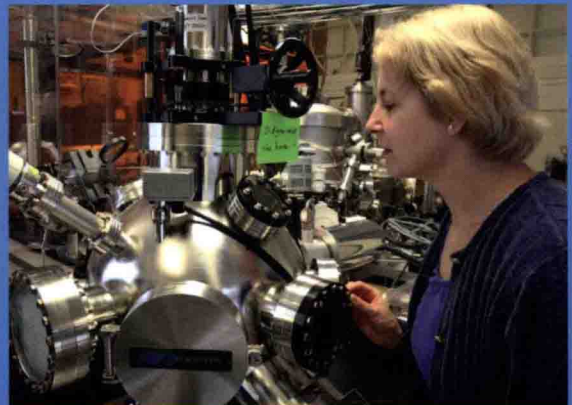
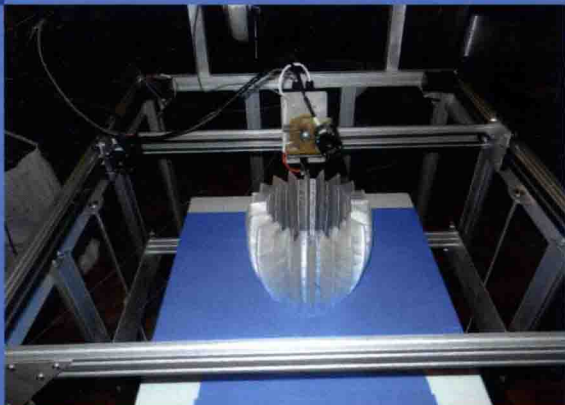


Materials Science and Engineering



Emilio McMahon

Materials Science and Engineering

The book aims to shed light on some of the unexplored aspects of materials science and engineering. It describes in detail the various concepts and theories of this field. Materials science refers to the study, design and discovery of new materials. This subject is used in different areas like nanotechnology, metallurgy, forensic engineering, biomaterials, and failure analysis, etc. This book is compiled in such a manner, that it will provide in-depth knowledge about the theory and practice of material science. The topics included in it are of utmost significance and bound to provide incredible insights to students. Some of the diverse topics covered in this book address the varied branches that fall under this category. This textbook is an essential guide for both graduates and post-graduates in this discipline.

Emilio McMahon holds a PhD. in Material Science and Engineering from College of Engineering, University of Kentucky, United States. He is actively engaged in the researches focused on biomaterials, metallurgy and ceramics. McMahon has been the recipient of two awards for his research work in the field of crystallography of polymers. He is an active member and a regular contributor to several scientific clubs and societies. He has also won an “Excellence in Graduate Education” award for his outstanding contribution towards the student community, especially in the undergraduate programs.



McMahon

Materials Science and Engineering

Larsen & Keller

Materials Science and Engineering

Edited by
Emilio McMahon

Materials Science and Engineering
Edited by Emilio McMahon
ISBN: 978-1-63549-177-7 (Hardback)

© 2017 Larsen & Keller

 Larsen & Keller

Published by Larsen and Keller Education,
5 Penn Plaza,
19th Floor,
New York, NY 10001, USA

Cataloging-in-Publication Data

Materials science and engineering / edited by Emilio McMahon.
p. cm.

Includes bibliographical references and index.

ISBN 978-1-63549-177-7

1. Materials science. 2. Materials. 3. Engineering.

4. Technology. I. McMahon, Emilio.

TA403 .M38 2017

620.11--dc23

This book contains information obtained from authentic and highly regarded sources. All chapters are published with permission under the Creative Commons Attribution Share Alike License or equivalent. A wide variety of references are listed. Permissions and sources are indicated; for detailed attributions, please refer to the permissions page. Reasonable efforts have been made to publish reliable data and information, but the authors, editors and publisher cannot assume any responsibility for the validity of all materials or the consequences of their use.

Trademark Notice: All trademarks used herein are the property of their respective owners. The use of any trademark in this text does not vest in the author or publisher any trademark ownership rights in such trademarks, nor does the use of such trademarks imply any affiliation with or endorsement of this book by such owners.

The publisher's policy is to use permanent paper from mills that operate a sustainable forestry policy. Furthermore, the publisher ensures that the text paper and cover boards used have met acceptable environmental accreditation standards.

Printed and bound in China.

For more information regarding Larsen and Keller Education and its products, please visit the publisher's website www.larsen-keller.com

Materials Science and Engineering



Preface

The book aims to shed light on some of the unexplored aspects of materials science and engineering. It describes in detail the various concepts and theories of this field. Materials science refers to the study, design and discovery of new materials. This subject is used in different areas like nanotechnology, metallurgy, forensic engineering, biomaterials, and failure analysis, etc. This book is compiled in such a manner, that it will provide in-depth knowledge about the theory and practice of material science. The topics included in it are of utmost significance and bound to provide incredible insights to students. Some of the diverse topics covered in this book address the varied branches that fall under this category. This textbook is an essential guide for both graduates and post-graduates in this discipline.

To facilitate a deeper understanding of the contents of this book a short introduction of every chapter is written below:

Chapter 1- Materials science studies different designs and materials. It includes elements of physics, chemistry and engineering. The chapter on materials science offers an insightful focus, keeping in mind the complex subject matter.

Chapter 2- The essential concepts of materials science are biomaterials, composite materials, acoustic emission, crystal growth, Hume-Rothery rules and hysteresis. Biomaterial is the substance that is made to interact with biological systems whereas a composite material is a material made from constituents that have different physical or chemical properties. The major components of materials science are discussed in this section.

Chapter 3- Aerogel is a material that is originated from a gel; the liquid constituent in the gel is substituted with a gas. Alternatively, the other emerging technologies in materials science are metamaterial, nanomaterial, programmable matter, quantum dot etc. The aspects elucidated in this text are of vital importance, and provide a better understanding of materials science.

Chapter 4- A crystal is a material that is in a proper structure. They can be recognized by their geometrical shape. The other atomic arrangements discussed in this chapter are crystal structure, Miller index, crystal structure prediction, crystallographic defect etc. This section serves as a source to understand the basic aspects of atomic arrangements present in solids.

Chapter 5- The bond between atoms and chemical compounds is known as chemical bonding. Ionic bonding, covalent bond, metallic bonding and electronegativity are other aspects of chemical bonding. This section is an overview of the subject matter incorporating all the major aspects of chemical bonding.

Chapter 6- Carbon nanotubes are allotropes of carbon. They have unusual properties and are very valuable for electronics, optics and nanotechnology. Topics such as optical properties of carbon nanotubes, synthesis of carbon nanotubes, carbon nanotube chemistry and selective chemistry of single-walled nanotubes have been explicated in the section.

Chapter 7- Metallurgy studies the physical and chemical behavior of metallic elements. It is the technology of metals. The process of working on these metals to create structures and assemblies is known as metalworking. The processes of metalworking that have been explained in this chapter are casting, forging, rolling, cladding, metal fabrication etc. This section elucidates the basic concepts of metallurgy.

Chapter 8- The allied fields of materials science are nanotechnology, polymer chemistry and radiation material science. Nanotechnology is the study of matter on atomic, molecular and supramolecular scale. This chapter helps the reader in developing an in depth understanding of all the fields that are allied to materials science.

I owe the completion of this book to the never-ending support of my family, who supported me throughout the project.

Editor

Table of Contents

	Preface	VII
Chapter 1	Introduction to Materials Science	1
Chapter 2	Essential Concepts of Materials Science	16
	a. Biomaterial	16
	b. Composite Material	20
	c. Acoustic Emission	72
	d. Crystal Growth	73
	e. Hume-Rothery Rules	80
	f. Hysteresis	80
Chapter 3	Atomic Arrangements in Solids	93
	a. Crystal	93
	b. Crystallography	100
	c. Amorphous Solid	105
	d. Crystal Structure	106
	e. Miller Index	116
	f. Crystallographic Defect	120
	g. Crystal Structure Prediction	125
Chapter 4	Emerging Technologies in Materials Science	128
	a. Aerogel	128
	b. High-temperature Superconductivity	136
	c. Metamaterial	149
	d. Nanomaterials	158
	e. Programmable Matter	164
	f. Quantum Dot	168
Chapter 5	Chemical Bonding: An Overview	193
	a. Chemical Bond	193
	b. Ionic Bonding	201
	c. Covalent Bond	205
	d. Metallic Bonding	209
	e. Electronegativity	215
	f. Intermolecular Force	223
Chapter 6	Carbon Nanotubes: An Integrated Study	228
	a. Carbon Nanotube	228
	b. Optical Properties of Carbon Nanotubes	240
	c. Synthesis of Carbon Nanotubes	249
	d. Carbon Nanotube Chemistry	255
	e. Selective Chemistry of Single-walled Nanotubes	259

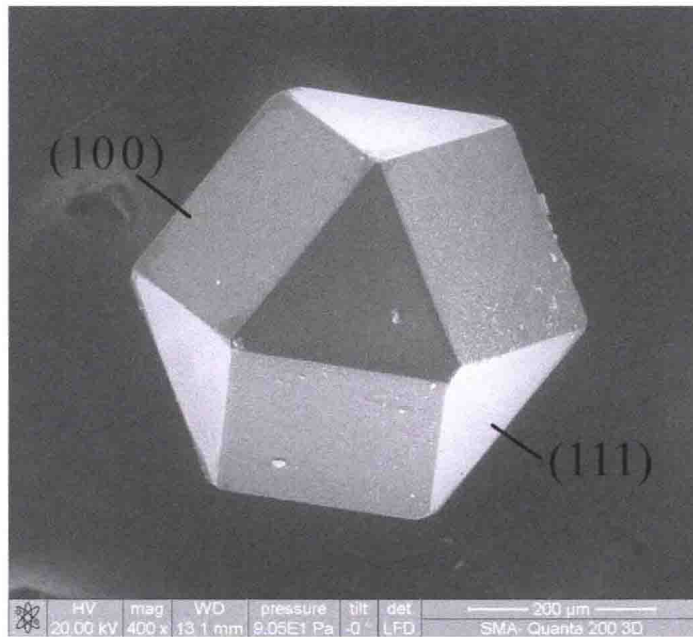
Chapter 7	Understanding Metallurgy	265
	a. Metallurgy	265
	b. Extractive Metallurgy	271
	c. Hydrometallurgy	274
	d. Metalworking	276
Chapter 8	Allied Fields of Materials Science	344
	a. Nanotechnology	344
	b. Polymer Chemistry	357
	c. Radiation Material Science	360

Permissions

Index

Introduction to Materials Science

Materials science studies different designs and materials. It includes elements of physics, chemistry and engineering. The chapter on materials science offers an insightful focus, keeping in mind the complex subject matter.



A diamond cuboctahedron showing seven crystallographic planes, imaged with scanning electron microscopy.

The interdisciplinary field of materials science, also commonly termed materials science and engineering, involves the discovery and design of new materials, with an emphasis on solids. The intellectual origins of materials science stem from the Enlightenment, when researchers began to use analytical thinking from chemistry, physics, and engineering to understand ancient, phenomenological observations in metallurgy and mineralogy. Materials science still incorporates elements of physics, chemistry, and engineering. As such, the field was long considered by academic institutions as a sub-field of these related fields. Beginning in the 1940s, materials science began to be more widely recognized as a specific and distinct field of science and engineering, and major technical universities around the world created dedicated schools of the study.

Materials science is a syncretic discipline hybridizing metallurgy, ceramics, solid-state physics, and chemistry. It is the first example of a new academic discipline emerging by fusion rather than fission.

Many of the most pressing scientific problems humans currently face are due to the limits of the materials that are available. Thus, breakthroughs in materials science are likely to affect the future of technology significantly.

Materials scientists emphasize understanding how the history of a material (its *processing*) influences its structure, and thus the material's properties and performance. The understanding of processing-structure-properties relationships is called the § materials paradigm. This paradigm is used to advance understanding in a variety of research areas, including nanotechnology, biomaterials, and metallurgy. Materials science is also an important part of forensic engineering and failure analysis - investigating materials, products, structures or components which fail or which do not operate or function as intended, causing personal injury or damage to property. Such investigations are key to understanding, for example, the causes of various aviation accidents and incidents.

History



A late Bronze Age sword or dagger blade.

The material of choice of a given era is often a defining point. Phrases such as Stone Age, Bronze Age, Iron Age, and Steel Age are great examples. Originally deriving from the manufacture of ceramics and its putative derivative metallurgy, materials science is one of the oldest forms of engineering and applied science. Modern materials science evolved directly from metallurgy, which itself evolved from mining and (likely) ceramics and the use of fire. A major breakthrough in the understanding of materials occurred in the late 19th century, when the American scientist Josiah Willard Gibbs demonstrated that the thermodynamic properties related to atomic structure in various phases are related to the physical properties of a material. Important elements of modern materials science are a product of the space race: the understanding and engineering of the metallic alloys, and silica and carbon materials, used in building space vehicles enabling the exploration of space. Materials science has driven, and been driven by, the development of revolutionary technologies such as rubbers, plastics, semiconductors, and biomaterials.

Before the 1960s (and in some cases decades after), many *materials science* departments were named *metallurgy* departments, reflecting the 19th and early 20th century emphasis on metals. The growth of materials science in the United States was catalyzed in part by the Advanced Research Projects Agency, which funded a series of university-hosted laboratories in the early 1960s "to expand the national program of basic research and training in the materials sciences." The field has since broadened to include every class of materials, including ceramics, polymers, semiconductors, magnetic materials, medical implant materials, biological materials, and nanomaterials.

Fundamentals

The materials paradigm represented in the form of a tetrahedron.

A material is defined as a substance (most often a solid, but other condensed phases can be included) that is intended to be used for certain applications. There are a myriad of materials around us—they can be found in anything from buildings to spacecraft. Materials can generally be divided into two classes: crystalline and non-crystalline. The traditional examples of materials are metals, semiconductors, ceramics and polymers. New and advanced materials that are being developed include nanomaterials and biomaterials, etc.

The basis of materials science involves studying the structure of materials, and relating them to their properties. Once a materials scientist knows about this structure-property correlation, they can then go on to study the relative performance of a material in a given application. The major determinants of the structure of a material and thus of its properties are its constituent chemical elements and the way in which it has been processed into its final form. These characteristics, taken together and related through the laws of thermodynamics and kinetics, govern a material's microstructure, and thus its properties.

Structure

As mentioned above, structure is one of the most important components of the field of materials science. Materials science examines the structure of materials from the atomic scale, all the way up to the macro scale. Characterization is the way materials scientists examine the structure of a material. This involves methods such as diffraction with X-rays, electrons, or neutrons, and various forms of spectroscopy and chemical analysis such as Raman spectroscopy, energy-dispersive spectroscopy (EDS), chromatography, thermal analysis, electron microscope analysis, etc. Structure is studied at various levels, as detailed below.

Atomic Structure

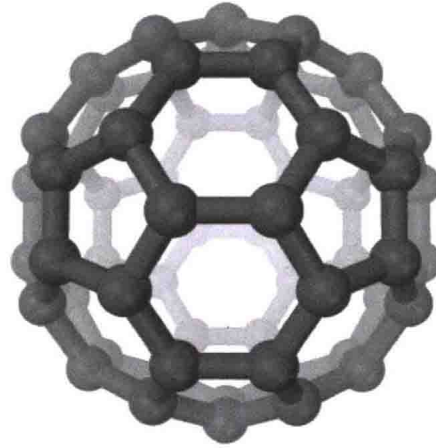
This deals with the atoms of the materials, and how they are arranged to give molecules, crystals, etc. Much of the electrical, magnetic and chemical properties of materials arise from this level of structure. The length scales involved are in angstroms. The way in which the atoms and molecules are bonded and arranged is fundamental to studying the properties and behavior of any material.

Nanostructure

Nanostructure deals with objects and structures that are in the 1–100 nm range. In many materials, atoms or molecules agglomerate together to form objects at the nanoscale. This causes many interesting electrical, magnetic, optical, and mechanical properties.

In describing nanostructures it is necessary to differentiate between the number of dimensions on the nanoscale. Nanotextured surfaces have *one dimension* on the nanoscale, i.e., only the thickness of the surface of an object is between 0.1 and 100 nm. Nanotubes have *two dimensions* on the nanoscale, i.e., the diameter of the tube is between 0.1 and 100 nm; its length could be much greater. Finally, spherical nanoparticles have *three dimensions* on the nanoscale, i.e., the particle is between 0.1 and 100 nm in each spatial dimension. The terms nanoparticles and ultrafine parti-

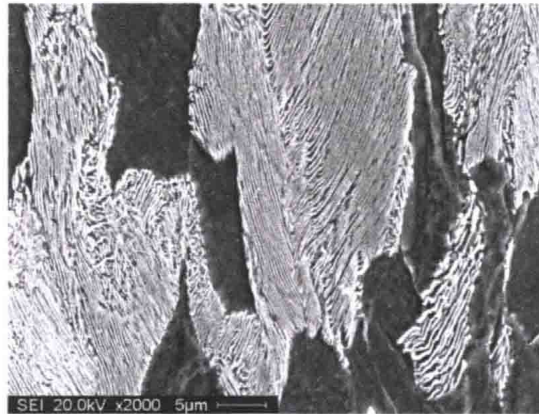
cles (UFP) often are used synonymously although UFP can reach into the micrometre range. The term 'nanostructure' is often used when referring to magnetic technology. Nanoscale structure in biology is often called ultrastructure.



Buckminsterfullerene nanostructure.

Materials which atoms and molecules form constituents in the nanoscale (i.e., they form nanostructure) are called nanomaterials. Nanomaterials are subject of intense research in the materials science community due to the unique properties that they exhibit.

Microstructure



Microstructure of pearlite.

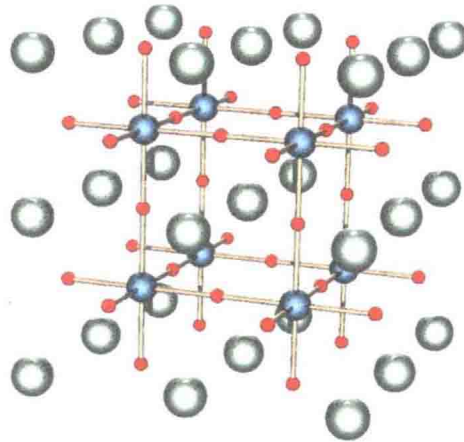
Microstructure is defined as the structure of a prepared surface or thin foil of material as revealed by a microscope above $25\times$ magnification. It deals with objects from 100 nm to a few cm. The microstructure of a material (which can be broadly classified into metallic, polymeric, ceramic and composite) can strongly influence physical properties such as strength, toughness, ductility, hardness, corrosion resistance, high/low temperature behavior, wear resistance, and so on. Most of the traditional materials (such as metals and ceramics) are microstructured.

The manufacture of a perfect crystal of a material is physically impossible. For example, a crystalline material will contain defects such as precipitates, grain boundaries (Hall–Petch relationship), interstitial atoms, vacancies or substitutional atoms. The microstructure of materials reveals these defects, so that they can be studied.

Macro Structure

Macro structure is the appearance of a material in the scale millimeters to meters—it is the structure of the material as seen with the naked eye.

Crystallography



Crystal structure of a perovskite with a chemical formula ABX_3 .

Crystallography is the science that examines the arrangement of atoms in crystalline solids. Crystallography is a useful tool for materials scientists. In single crystals, the effects of the crystalline arrangement of atoms is often easy to see macroscopically, because the natural shapes of crystals reflect the atomic structure. Further, physical properties are often controlled by crystalline defects. The understanding of crystal structures is an important prerequisite for understanding crystallographic defects. Mostly, materials do not occur as a single crystal, but in polycrystalline form, i.e., as an aggregate of small crystals with different orientations. Because of this, the powder diffraction method, which uses diffraction patterns of polycrystalline samples with a large number of crystals, plays an important role in structural determination. Most materials have a crystalline structure, but some important materials do not exhibit regular crystal structure. Polymers display varying degrees of crystallinity, and many are completely noncrystalline. Glass, some ceramics, and many natural materials are amorphous, not possessing any long-range order in their atomic arrangements. The study of polymers combines elements of chemical and statistical thermodynamics to give thermodynamic and mechanical, descriptions of physical properties.

Bonding

To obtain a full understanding of the material structure and how it relates to its properties, the materials scientist must study how the different atoms, ions and molecules are arranged and bonded to each other. This involves the study and use of quantum chemistry or quantum physics. Solid-state physics, solid-state chemistry and physical chemistry are also involved in the study of bonding and structure.

Properties

Materials exhibit myriad properties, including the following.

- Mechanical properties
- Chemical properties
- Electrical properties
- Thermal properties
- Optical properties
- Magnetic properties

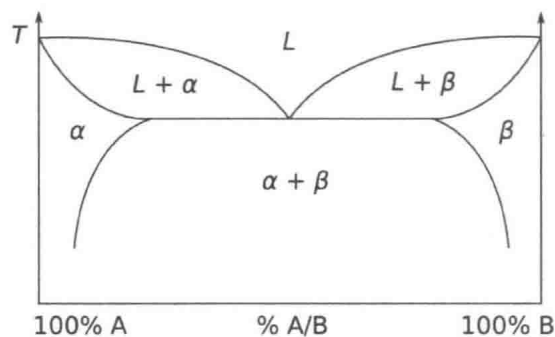
The properties of a material determine its usability and hence its engineering application.

Synthesis and Processing

Synthesis and processing involves the creation of a material with the desired micro-nanostructure. From an engineering standpoint, a material cannot be used in industry if no economical production method for it has been developed. Thus, the processing of materials is vital to the field of materials science.

Different materials require different processing or synthesis methods. For example, the processing of metals has historically been very important and is studied under the branch of materials science named *physical metallurgy*. Also, chemical and physical methods are also used to synthesize other materials such as polymers, ceramics, thin films, etc. As of the early 21st century, new methods are being developed to synthesize nanomaterials such as graphene.

Thermodynamics



A phase diagram for a binary system displaying a eutectic point.

Thermodynamics is concerned with heat and temperature and their relation to energy and work. It defines macroscopic variables, such as internal energy, entropy, and pressure, that partly describe a body of matter or radiation. It states that the behavior of those variables is subject to general constraints, that are common to all materials, not the peculiar properties of particular materials. These general constraints are expressed in the four laws of thermodynamics. Thermodynamics describes the bulk behavior of the body, not the microscopic behaviors of the very large numbers of its microscopic constituents, such as molecules. The behavior of these microscopic particles is described by, and the laws of thermodynamics are derived from, statistical mechanics.