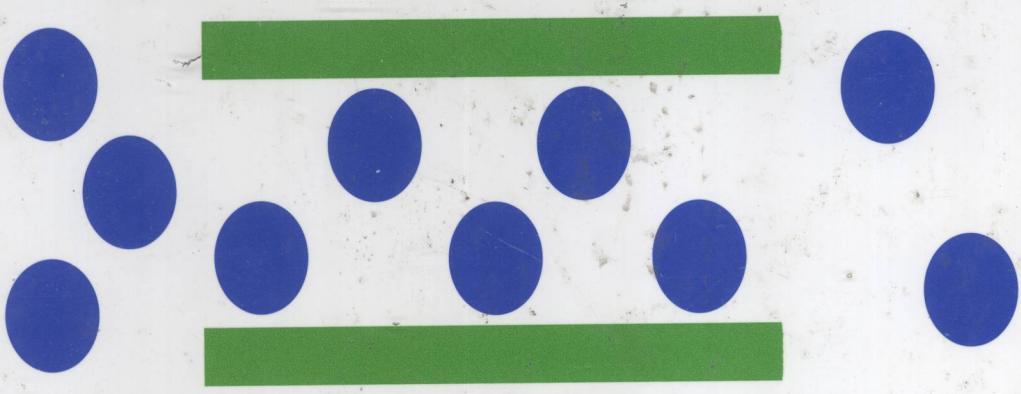
Adsorption and Diffusion in Nanoporous Materials



Rolando M.A. Roque-Malherbe

CRC Press
Taylor & Francis Group

TB383
R786

Adsorption and Diffusion in Nanoporous Materials

Rolando M.A. Roque-Malherbe

CRC Press
Taylor & Francis Group
Boca Raton London New York

CRC Press is an imprint of the
Taylor & Francis Group, an informa business

CRC Press
Taylor & Francis Group
6000 Broken Sound Parkway NW, Suite 300
Boca Raton, FL 33487-2742

© 2007 by Taylor & Francis Group, LLC
CRC Press is an imprint of Taylor & Francis Group, an Informa business

No claim to original U.S. Government works
Printed in the United States of America on acid-free paper
10 9 8 7 6 5 4 3 2 1

International Standard Book Number-10: 1-4200-4675-6 (Hardcover)
International Standard Book Number-13: 978-1-4200-4675-5 (Hardcover)

This book contains information obtained from authentic and highly regarded sources. Reprinted material is quoted with permission, and sources are indicated. A wide variety of references are listed. Reasonable efforts have been made to publish reliable data and information, but the author and the publisher cannot assume responsibility for the validity of all materials or for the consequences of their use.

No part of this book may be reprinted, reproduced, transmitted, or utilized in any form by any electronic, mechanical, or other means, now known or hereafter invented, including photocopying, microfilming, and recording, or in any information storage or retrieval system, without written permission from the publishers.

For permission to photocopy or use material electronically from this work, please access www.copyright.com (http://www.copyright.com/) or contact the Copyright Clearance Center, Inc. (CCC) 222 Rosewood Drive, Danvers, MA 01923, 978-750-8400. CCC is a not-for-profit organization that provides licenses and registration for a variety of users. For organizations that have been granted a photocopy license by the CCC, a separate system of payment has been arranged.

Trademark Notice: Product or corporate names may be trademarks or registered trademarks, and are used only for identification and explanation without intent to infringe.

Library of Congress Cataloging-in-Publication Data

Roque-Malherbe, Rolando M.A.
Adsorption and diffusion in nanoporous materials / author/editor (s) Rolando M.A. Roque-Malherbe.
p. cm.
Includes bibliographical references and index.
ISBN-13: 978-1-4200-4675-5 (alk. paper)
ISBN-10: 1-4200-4675-6 (alk. paper)
1. Porous materials. 2. Nanostructured materials. 3. Diffusion. 4. Adsorption. I. Title.

TA418.9.P6R67 2007
620.1'16--dc22 2006030712

Visit the Taylor & Francis Web site at
http://www.taylorandfrancis.com

and the CRC Press Web site at
http://www.crcpress.com

Adsorption and Diffusion in Nanoporous Materials

Dedication

This book is dedicated to my mother, Silvia;
my father, Rolando; my wife, Teresa; our sons, Edelin,
Rolando, Ruben, and Daniel; our grandchildren,
Sarah, Rolando, Natalie, and Nicolas; and
all our pets, very especially to Zeolita and Trosia.

此为试读,需要完整PDF请访问: www.ertongbook.com

Preface

The increase in the concentration of molecules from a gaseous phase in the neighboring solid surface was recognized in 1777 by Fontana and Scheele, and the term ***ADSORPTION*** to describe the effect was coined by Kayser in 1881. On the other hand, ***DIFFUSION*** is a general property of matter related to the tendency of a system to occupy all its accessible states. The quantitative study of this phenomenon started in 1850–1855 with the works of Adolf Fick and Thomas Graham.

The development of new materials is a basic objective of materials science research. This interest is fueled by the progress in all fields of industry and technology. For example, the evolution of the electronic industry initiated the development of smaller and smaller elements. The size of these components is approaching nanometer dimensions, and as this dominion is entered, scientists have found that properties of materials with nanometer dimensions, i.e., on the length scale of about 1–100 nm, can differ from those of the bulk material. In these dimensions, adsorption and diffusion are important methods of characterization. They are processes that determine the governing laws of important fields of application of nanoporous materials.

According to the definition of the International Union of Pure and Applied Chemistry (IUPAC), ***POROUS MATERIALS*** are classified as microporous materials, which are those with pore diameters between 0.3 and 2 nm; mesoporous materials; which are those that have pore diameters between 2 and 50 nm, and macroporous materials; which are those with pores bigger than 50 nm. Within the class of porous materials, nanoporous materials, such as zeolites and related materials, mesoporous molecular sieves, the majority of silica, and active carbons are the most widely studied and applied. In the cases of crystalline and ordered nanoporous material such as zeolites and related materials and mesoporous molecular sieves, classification as nanoporous materials is not discussed. However, amorphous porous materials may possess, together with pores with sizes less than 100 nm, larger pores. Even in this case, in the majority of instances, the nanoporous component is the most important part of the porosity.

Adsorption and diffusion have a manifold value, since they are not only powerful means for the characterization of nanopoorus materials but are also important industrial operations. The adsorption of a gas can bring information of the microporous volume, the mesopore area, the volume and size of the pores, and the heat of adsorption. On the other hand, diffusion controls the molecular transport of gases in porous media and also brings morphological information, in the case of amorphous materials, and structural information, in the case of crystalline and ordered materials.

Crystalline, ordered, and amorphous microporous and mesoporous materials, such as microporous and mesoporous molecular sieves, amorphous silica and alumina, active carbons, and other materials obtained by different techniques, are the source

of a collection of advanced materials with exceptional properties and applications in many fields such as optics, electronics, ionic conduction, ionic exchange, gas separation, membranes, coatings, catalysts, catalysts supports, sensors, pollution abatement, detergency, and biology.

This book is derived from some of the author's previous books, chapters of books, and papers. The author has tried to present a state-of-the-art description of some of the most important aspects of the **THEORY** and **PRACTICE** of adsorption and diffusion, fundamentally of gases in microporous crystalline, mesoporous ordered, and micro/mesoporous amorphous materials.

The adsorption process in multicomponent systems will not be discussed in this book with the exception of the final chapter, which analyzes adsorption from the liquid phase. Fundamentally, we are studying adsorption and diffusion from the point of view of materials science. That is, we are interested in the methods for the use of single-component adsorption and diffusion in the characterization of the adsorbent surface, pore volume, pore size distribution, and the study of the parameters characterizing single-component transport processes in porous systems. Also studied in the text are: adsorption energetic, adsorption thermodynamics, and dynamic adsorption in plug-flow bed reactors. The structure or morphology and the methods of synthesis and modification of silica, active carbons, zeolites and related materials, and mesoporous molecular sieves are discussed in the text as well. Other adsorbents normally used in different applications, such as alumina, titanium dioxide, magnesium oxide, clays, and pillared clays are not discussed.

From the point of view of the application of dynamic adsorption systems, the author will analyze the use of adsorbents to clean gas or liquid flows by the removal of a low-concentration impurity, applying a plug-flow adsorption reactor (PFAR) where the output of the operation of the PFAR is a breakthrough curve.

Finally, the book is dedicated to my family. It is also devoted to the advisors of my postgraduate studies and the mentors in my postdoctoral fellowships. In particular, I would like to recognize Dr. Professor Jürgen Büttner, advisor of my M.Sc. studies, who was the first to explain to me the importance of the physics and chemistry of surfaces in materials science. I would like also to acknowledge my senior Ph.D. tutor, the late Professor Alekzander A. Zhujovistskii, who, in 1934, was the first to recognize the complementary role of the adsorption field and capillary condensation in adsorption in porous materials and was later one of the creators of gas chromatography. He taught me how to "see" inside scientific data using general principles. Also, I wish to recognize my junior Ph.D. tutor, Professor Boris S. Bokstein, a well-know authority in the study of transport phenomena, who motivated me to study diffusion. I want, as well, to acknowledge the mentors of my postdoctoral fellowships, Professor Fritz Storbeck, who gave me the opportunity to be in contact with the most advanced methods of surface studies; Professor Evgenii D. Shchukin, one of the creators of a new science, physicochemical mechanics, who taught me the importance of surface phenomena in materials science; and the late academic Mijail M. Dubinin and Professor A.V. Kiseliov, two of the most important scientists in the field of adsorption science and technology during the last century. Both of

them gave me the opportunity to more deeply understand their philosophy of adsorption systems.

Professor Rolando M.A. Roque-Malherbe, Ph.D.
Las Piedras, Puerto Rico, USA

Author

Professor Rolando M.A. Roque-Malherbe was born in 1948 in Güines, Havana, Cuba. He finished his B.S. in physics at Havana University (1970), his specialization (M.S. equivalent degree) in surface physics in the National Center for Scientific Research–Technical University of Dresden, Germany (1972), and his Ph.D. in physics at the Moscow Institute of Steel and Alloys, Russia (1978). He completed postdoctoral stays at the Technical University of Dresden, Moscow State University, Technical University of Budapest, and the Institute of Physical Chemistry and Central Research Institute for Chemistry of the Russian and Hungarian Academies of Science (1978–1984). Professor Roque-Malherbe headed a research group in the National Center for Scientific Research–Higher Pedagogical Institute in Varona, Havana, Cuba (1980–1992), which is a world leader in the study and application of natural zeolites. In 1993, after a confrontation with the Cuban regime, he left Cuba with his family as a political refugee. From 1993 to 1999, he worked at the Institute of Chemical Technology, Valencia, Spain; Clark Atlanta University, Atlanta, Georgia; and Barry University, Miami, Florida. From 1999 to 2004 he was dean and full professor of the School of Science at Turabo University (TU), Gurabo, Puerto Rico, and currently is the Director of the Institute of Physico-Chemical Applied Research at TU. He has published 112 papers, 3 books, 5 chapters, 15 patents, 29 abstracts, and has given more than 200 presentations at scientific conferences. He is currently an American citizen.

Table of Contents

Chapter 1 Statistical Mechanics 1

1.1 Introduction 1
1.1.1 Thermodynamic Functions and Relationships 1
1.2 Definition of Microstate and Macrostate 2
1.3 Definition of Ensemble 4
1.4 The Canonical Ensemble 5
1.5 Evaluation of α and β for the Canonical Ensemble 8
1.6 The Grand Canonical Ensemble 9
1.7 Evaluation of α, β, and γ for the Grand Canonical Ensemble 11
1.8 Canonical Partition Function for a System of Noninteracting Particles 13
1.9 Factorization of the Molecular Partition Function 15
1.10 Density Functional Theory (DFT) 16
1.11 Thermodynamics of Irreversible Processes 20
1.12 Statistical Mechanics of Irreversible Processes 23
1.12.1 Correlation Functions and Generalized Susceptibilities 24
1.12.2 Calculation of the Mean Square Displacement and the Self-Diffusion Coefficient 26
1.12.2.1 Calculation of the Mean Square Displacement with the Help of the Velocity Autocorrelation Function 26
1.12.2.2 Langevin's Brownian Motion Model 27
1.12.2.3 The Diffusion Equation 29
References 31
Appendix 1.1 Legendre Transformations 33
Appendix 1.2 The Lagrange Multipliers 33
Appendix 1.3 Methods of Counting 35
Appendix 1.4 Calculus of Variations 36

Chapter 2 General Introduction to Adsorption in Solids 39

2.1 Definitions and Terminology 39
2.1.1 What Is the Meaning of the Term Adsorption 39
2.1.2 Phases and Components Involved in the Adsorption Process 39
2.1.3 Porous Materials 40
2.2 Interfacial Layer, Gibbs Dividing Surface, and Gibbs Adsorption 41
2.3 Thermodynamics of Gas–Solid Adsorption 43
2.3.1 Adsorption Interaction Fields 43
2.3.2 Isosteric and Differential Heats of Adsorption 44
2.3.3 Some Relations between Adsorption Macroscopic and Microscopic Parameters 46

2.4 Gases and Vapors Adsorption in Porous Materials 47
2.4.1 Measurement of Adsorption Isotherms by the Volumetric Method 47
2.4.2 Porous Materials Characterization by Vapor Adsorption Methods 49
2.5 Some Examples of the Application of the Volumetric Method 50
2.5.1 Volumetric Automatic Surface Area and Porosity Measurement Systems 50
2.5.2 Adsorption Isotherms of Nitrogen at 77 K in Zeolites 52
2.5.3 Calorimetry of Adsorption of NH_3 in $AlPO_4$-5 and FAPO-5 Molecular Sieves 53
References 54

Chapter 3 Microporosity and Surface Area Evaluation Methods 57

3.1 Introduction 57
3.2 The Dubinin and Osmotic Adsorption Isotherms 57
3.2.1 Dubinin Adsorption Isotherm 57
3.2.2 Osmotic Adsorption Isotherm 61
3.3 Langmuir and Fowler–Guggenheim Type Adsorption Isotherm Equations 63
3.3.1 Introduction 63
3.3.2 Application of the Grand Canonical Ensemble Methodology to Describe Adsorption in Zeolites 64
3.3.2.1 Immobile Adsorption 65
3.3.2.2 Mobile Adsorption 68
3.3.3 Some Remarks in Relation with the Langmuir Type and Fowler–Guggenheim Type Adsorption Isotherm Equations 69
3.4 The t-Plot Method 72
3.5 Additional Comments about the Application of the Dubinin and Osmotic Isotherms, the LT and the FGT Isotherm Equation Types, and the t-Plot Method in the Measurement of the Micropore Volume 76
3.6 The BET Method 79
3.7 Horvath-Kawazoe Method 85
References 89

Chapter 4 Nanoporous Materials Mesoporosity Evaluation 93

4.1 Introduction 93
4.2 Capillary Condensation 93
4.3 Macroscopic Theories to Describe Pore Condensation 96
4.3.1 The Kelvin-Cohan Equation 96
4.3.2 The Derjaguin-Broeckhoff-de Boer Theory 102
4.3.3 Some Concluding Remarks about the Macroscopic Theories to Describe Multilayer Adsorption and Pore Condensation 105

此为试读,需要完整PDF请访问: www.ertongbook.com

4.4 Density Functional Theory 106
4.4.1 The Density Functional Theory Methodology in General 106
4.4.2 Calculation of the Pore Size Distribution 108
4.4.3 The Nonlocal Density Functional Theory for the Description of Adsorption in Slit Pores, Cylindrical Pores, and Spherical Cavities 109
4.4.4 Some Concluding Remarks about the Molecular Models to Describe Adsorption 117
References 119

Chapter 5 Diffusion in Porous Materials 121

5.1 Introduction 121
5.2 Fick's Laws 121
5.3 Transport, Self-Diffusion, and Corrected Coefficients 123
5.3.1 Transport Diffusion and Self-Diffusion 123
5.3.2 Interdiffusion and the Frame of Reference for Porous Materials 124
5.3.3 Relation between the Transport, D, the Corrected, D_0, and the Diffusion Coefficients 125
5.3.4 Relation between the Transport, D, the Corrected, D_0, and the Self-Diffusion Coefficients in Zeolites 126
5.4 Mean Square Displacement, the Random Walker, and Gaseous Diffusion 127
5.4.1 The Mean Square Displacement (MSD) 127
5.4.2 Gaseous Diffusion and the Random Walker 128
5.5 Transport Mechanisms in Porous Media 130
5.6 Viscous, Knudsen, and Transition Flows 132
5.7 Viscous and Knudsen Flows in Model Porous Systems 134
5.7.1 Viscous Flow in a Straight Cylindrical Pore 134
5.7.2 Knudsen Flow in a Straight Cylindrical Pore 135
5.8 Transport in Real Porous Systems: Membranes 136
5.8.1 Membranes 136
5.8.2 Permeation Mechanisms in Porous Membranes 137
5.8.3 Viscous Flow in Membranes 139
5.8.4 Knudsen Flow in Membranes 140
5.8.5 Transition Flow 141
5.8.6 Surface Flow in the Adsorbed Phase 142
5.8.7 Experimental Permeation Study of Zeolite-Based Porous Ceramic Membranes 143
5.9 Diffusion in Microporous Materials: Zeolites and Related Materials 146
5.9.1 Model Description of Molecular Diffusion in Zeolites and Related Materials 147
5.9.2 Anomalous Diffusion 152
5.9.3 Experimental Methods for the Study of Diffusion in Zeolites 155
References 163

Chapter 6 The Plug-Flow Adsorption Reactor 167

6.1 Dynamic Adsorption 167
6.2 The Plug-Flow Adsorption Reactor Model 169
References 175
Appendix 6.1 Laplace Transforms 176

Chapter 7 Amorphous Porous Adsorbents: Silica and Active Carbon 181

7.1 Basic Features of Amorphous Silica 181
7.2 Amorphous Silica Morphology and Surface Chemistry 182
7.3 Precipitated Amorphous Silica Synthesis 185
7.4 Silica Modification 188
7.5 Fundamental Characteristics of Active Carbon 190
7.6 Active Carbon Morphology, Surface Chemistry, and Surface Modification 191
7.7 Active Carbon Production Methods 193
7.8 Some Applications of Precipitated Silica in Gas Phase Adsorption Processes 195
7.8.1 Adsorption of NH_3, H_2O, CO, N_2O, CO_2, and SH_2 in Precipitated Silica 195
7.8.2 Application of Precipitated Silica in Hydrogen Storage 197
7.8.3 Adsorption of Volatile Organic Compounds (VOCs) in Precipitated Silica 198
7.9 Some Applications of Activated Carbons and Other Carbonaceous Materials in Gas-Phase Adsorption Processes 199
7.9.1 Adsorption of H_2O and CO_2 and Removal of SH_2 and SO_2 with Active Carbon 199
7.9.2 Hydrogen Storage with Active Carbon and Other Carbonaceous Materials 202
7.9.3 Methane Storage in Activated Carbon and Other Carbonaceous Materials 202
7.9.4 Adsorption of Volatile Organic Compounds (VOCs) in Activated Carbon 203
7.9.5 Air-Conditioning with Activated Carbon 204
References 204

Chapter 8 Crystalline and Ordered Nanoporous Materials 211

8.1 Introduction 211
8.2 Fundamental Characteristics of Zeolites and Mesoporous Molecular Sieves 212
8.3 Structure 213
8.3.1 Crystalline Microporous Materials 213
8.3.2 Ordered Mesoporous Materials 216

8.4 Synthesis and Modification 219
8.4.1 Zeolite Synthesis 219
8.4.2 Zeolite Modification 222
8.4.3 Synthesis of Ordered Silica Mesoporous Materials 223
8.4.4 Modification of Ordered Silica Mesoporous Materials 225
8.5 Some Applications of Crystalline and Ordered Nanoporous Materials in Gas Separation and Adsorption Processes 227
8.5.1 Gas Cleaning 227
8.5.1.1 Zeolites 227
8.5.1.2 Mesoporous Molecular Sieves 230
8.5.2 Pressure Swing Adsorption 232
8.5.3 Other Separation Applications 233
8.5.4 Air-Conditioning 234
References 235

Chapter 9 Adsorption from Liquid Solution 243

9.1 Introduction 243
9.2 Surface Excess Amount and Amount of Adsorption for Liquid–Solid Adsorption Systems 244
9.3 Empirical Adsorption Isotherms Applied for the Correlation of Liquid–Solid Adsorption Equilibria in Systems Containing One Dissolved Component 247
9.4 Model Description of Adsorption from the Liquid Phase on Solids 250
9.5 Some Applications of Liquid–Solid Adsorption 252
9.5.1 Activated Carbons 252
9.5.2 Precipitated Silica 253
9.5.3 Zeolites 255
References 255

Index 259

1 Statistical Mechanics

1.1 INTRODUCTION

Statistical mechanics, or statistical physics, also named statistical thermodynamics in equilibrium systems, was originated in the work of Maxwell and Boltzmann on the kinetics theory of gases (1860–1900) [1–11]. Later, in his book *Elementary Principles of Statistical Physics,* Gibbs (1902) made a major advance in the theory and methods of calculation. In the twentieth century, Einstein, Fermi, Bose, Tolman, Langmuir, Landau, Fowler, Guggenheim, Kubo, Hill, Bogoliubov, and others contributed to the subsequent development and fruitful application of statistical mechanics [1–11].

Statistical mechanics deals with macroscopic systems, which consist of a collection of particles, for example, photons, electrons, atoms, or molecules, with composition, structure, and function. In statistical mechanics the term state has two meanings: the microstate, or quantum state, and the macrostate, or thermodynamic state.

1.1.1 Thermodynamic Functions and Relationships

Statistical physics, as will be shown in the present chapter, is a very comprehensive methodology for the calculation, for example, of the thermodynamic functions characterizing a macroscopic system. The fundamental equation of thermodynamics for a bulk mixture (i.e., a number of components included in the same homogeneous phase is [1,2]:

$$dU = TdS - PdV + \sum_i \mu_i dn_i$$

where $U(S,V,n_i)$ is the internal energy of the system; S, its entropy; V, its volume; T, its temperature; μ_i, the chemical potentials; and n_i, the number of moles, of one of the N components which form the system.

Similarly, using the Legendre transformations (see Appendix 1.1), by which the product of the substituted variables, in the present case, TS will be subtracted:

$$F = U - TS$$

one gets a new thermodynamic function, in the present case, $F(T,V,n_i)$, the Helmholtz free energy.

At this point, an additional thermodynamic function, the enthalpy, could also be defined [1,2]:

$$H = U + PV.$$

After that, the Gibbs function, or free enthalpy, is also obtained, with the help of the Legendre transformation [1,2]:

$$G = H - TS$$

It is also possible to define the grand potential, or Massieu function [10]:

$$\Omega = F - \sum \mu_i n_i$$

Subsequently, the corresponding set of differential equations for a bulk mixture are [1,2,10]:

$$dF = -SdT - PdV + \sum_i \mu_i dn_i$$

$$d\Omega = -SdT - PdV - \sum_i n_i d\mu_i$$

$$dH = TdS - VdP + \sum_i \mu_i dn_i$$

$$dG = -SdT + VdP + \sum_i \mu_i dn_i$$

The grand potential, which is generally absent from textbooks on thermodynamics, has a particular meaning in statistical thermodynamics. It is the thermodynamic potential for a system with fixed volume, V, chemical potentials, μ_i, and temperature, T, and as will be later shown, is related to the grand canonical partition, which is one of the magnitudes calculated with the help of the methods of statistical thermodynamics.

Table 1.1 reports some thermodynamic relations [10].

1.2 DEFINITION OF MICROSTATE AND MACROSTATE

A **microstate** is defined as a state of the system where all the parameters of the component particles are specified [7]. In quantum mechanics, in a system in a stationary state the energy levels and the state of the particles in terms of quantum numbers are used to specify the parameters of a microstate. At any given time the

TABLE 1.1
Thermodynamic Relations

$T=\left(\frac{\partial U}{\partial S}\right)_{V,n_i}$	$-P=\left(\frac{\partial U}{\partial V}\right)_{S,n_i}$	$\mu_i=\left(\frac{\partial U}{\partial n_i}\right)_{S,V,n_j(j\neq i)}$
$-S=\left(\frac{\partial F}{\partial T}\right)_{V,n_i}$	$-P=\left(\frac{\partial F}{\partial V}\right)_{T,n_i}$	$\mu_i=\left(\frac{\partial F}{\partial n_i}\right)_{T,V,n_j(j\neq i)}$
$T=\left(\frac{\partial H}{\partial T}\right)_{P,n_i}$	$V=\left(\frac{\partial H}{\partial P}\right)_{S,n_i}$	$\mu_i=\left(\frac{\partial H}{\partial n_i}\right)_{S,P,n_j(j\neq i)}$
$-S=\left(\frac{\partial G}{\partial T}\right)_{P,n_i}$	$V=\left(\frac{\partial G}{\partial P}\right)_{T,n_i}$	$\mu_i=\left(\frac{\partial G}{\partial n_i}\right)_{T,P,n_j(j\neq i)}$
$-S=\left(\frac{\partial \Omega}{\partial T}\right)_{V,\mu_i}$	$-P=\left(\frac{\partial \Omega}{\partial P}\right)_{T,\mu_i}$	$-n_i=\left(\frac{\partial \Omega}{\partial \mu_i}\right)_{T,V,n_i(i\neq j)}$

system will be in a definite quantum state, *j*, characterized by a certain wave function, φ_j, which is a function of a huge number of spatial and spin coordinates, an energy, E_j, and a set of quantum numbers [7].

A **macrostate** is defined as a state of the system where the distribution of particles over the energy levels is specified [7]. The macrostate includes different energy levels and particles having particular energies. That is, it contains many microstates. However, following the principles of thermodynamics [1,2], it is known that, for a single component system, we only need to designate three macroscopic parameters, i.e., *(P,V,T)*, *(P,V,N)*, or *(E,V,N)*, where *P is* pressure, *V is* volume, *T is* temperature, and *N* is the number of particles, in order to specify the thermodynamic state of an equilibrium single-component system. In this case, the equation of state for the system relates the three variables to a fourth. For example, for an ideal gas we have:

$$PV = nRT = NkT.$$

in which $R = 8.31451$ [$JK^{-1}mol^{-1}$] is the ideal gas constant, where $R = N_A k$, in which $N_A = 6.02214 \times 10^{23}$ [mol^{-1}] is the Avogadro number, and $k = 1.38066$ [JK^{-1}], is the Boltzmann constant.

In an ideal gas, we assume that the molecules are noninteracting, i.e., they do not affect each other's energy levels. Each particle possesses a certain energy, and at $T > 0$, the system possesses a total energy, E. From quantum mechanics, we know that the possible energies, if we consider the particles confined in a cubic box of volume, $V = abc$ (see Figure 1.1), are [8]:

$$E(n_1,n_2,n_3)=\frac{h^2}{8m}\left(\frac{n_1^2}{a^2}+\frac{n_2^2}{b^2}+\frac{n_3^2}{c^2}\right)$$

此为试读,需要完整PDF请访问: www.ertongbook.com