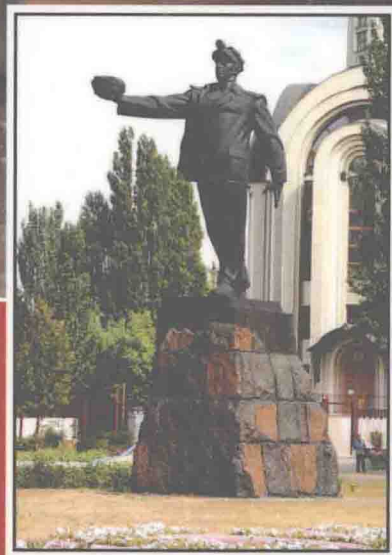
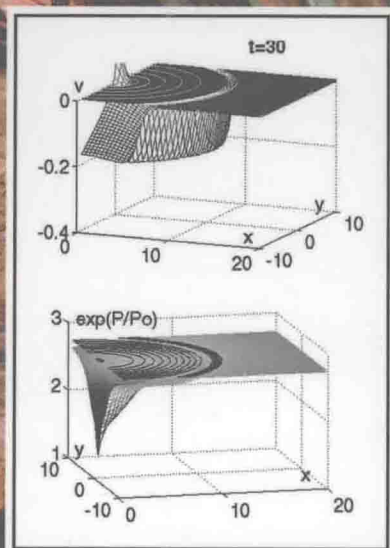


PHYSICS OF COAL AND MINING PROCESSES



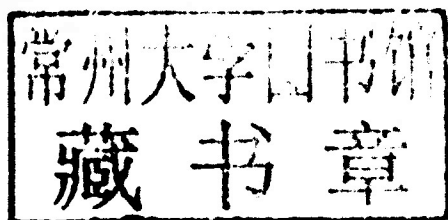
Anatoly D. Alexeev



CRC Press
Taylor & Francis Group

PHYSICS OF COAL AND MINING PROCESSES

Anatoly D. Alexeev



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

© 2012 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
Version Date: 20111020

International Standard Book Number: 978-1-4398-7634-3 (Hardback)

This book contains information obtained from authentic and highly regarded sources. Reasonable efforts have been made to publish reliable data and information, but the author and publisher cannot assume responsibility for the validity of all materials or the consequences of their use. The authors and publishers have attempted to trace the copyright holders of all material reproduced in this publication and apologize to copyright holders if permission to publish in this form has not been obtained. If any copyright material has not been acknowledged please write and let us know so we may rectify in any future reprint.

Except as permitted under U.S. Copyright Law, 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

Alexeev, Anatoly D.
Physics of coal and mining processes / Anatoly D. Alexeev.
p. cm.
Includes bibliographical references and index.
ISBN 978-1-4398-7634-3 (hardcover : alk. paper)
1. Coal mines and mining--Ukraine. 2. Mining engineering--Ukraine. I. Title.

TN808.U4A44 2012
622'.33409477--dc23

2011038367

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

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

Foreword

Coal represents the wealth of Ukraine and ensures the nation's energy independence to a considerable extent. Therefore, increasing coal production is a very important strategic objective for our future. Unfortunately, the coal industry is often connected with loss of human lives. The National Academy of Sciences of Ukraine implements regular basic studies in the physics of coal and physics of mining processes to enhance our understanding of the nature of methane emissions in mines and provide the safest mining conditions.

This book is an exhaustive monograph summarizing physical approaches to coal beds (including deep beds) and coals as complex physical media based on fundamental experimental and theoretical studies conducted at the Institute for Physics of Mining Processes of the National Academy of Sciences of Ukraine (Donetsk) headed by Anatoly D. Alexeev, the author and a corresponding member of the Academy. These studies focused on analyses of coal structures using radiophysical methods such as nuclear magnetic and electronic paramagnetic resonances; discovery of phase states of methane in coals and methane solubility in less matured coals; observations of methane mass transfer in coal-methane systems; and many other relevant topics. Results of these studies obtained using modern equipment made it possible to implement novel methods of coal bed behavior prediction and develop measures to prevent highly explosive coal and gas outbursts, with the primary goal of increasing worker safety in Ukraine mines.

I am sure that the publication of *Physics of Coal and Mining Processes* will be an important event for all specialists interested in coal mining and will introduce them to the achievements of Ukrainian scientists in this important field.

B. E. Paton

President of National Academy of Sciences of Ukraine

Preface

The physics of mining processes is a relatively new branch of science that evolved to solve problems arising during mineral products recovery (this volume concentrates on coal), particularly safety issues such as prevention of rock failures, coal and gas outbursts, and methane explosions. Around the globe, on average, four coal miners die for each million tons of coal recovered. Substantially increasing coal production and improving the safety of mining work are impossible without further development of the physics of mining processes. The main mission of the Institute for Physics of Mining Processes of the National Academy of Sciences of Ukraine established in 2003 is to serve the needs of the Ukrainian major coal mining industry.

This volume discusses research work carried out at the institute and information gathered from international observations. It includes chapters relating to massif mechanics. I found it reasonable to include a chapter addressing the most important safety issues such as control of coal and gas outbursts and estimates for accumulation times of explosive methane concentrations in different phase states (adsorbates on surfaces, solid solutions in coal, etc.). Solutions to the specified problems may be found in research discoveries in coal physics and the physics of mining processes.

Most studies on the physics of mining processes are dedicated to specific critical problems. This study is the first to present a unifying methodology for addressing various problems arising in the mining industry. Concentrating on the key issue of each particular problem, I discuss the adopted assumptions and approximations and apply the fundamental laws of physics. The reader will easily recognize the unity of the approaches used. In each case, the validity criterion of the adopted model is the solution of a particular industrial problem.

Because of the vital importance of mineral products recovery for modern industry, the physics of coal and mining processes has been rapidly developing around the world for decades. I attempt to cover the main discoveries and achievements to the fullest extent possible because I have not found a general study of the subject in the research literature. The reader will find many original results along with discussions and development of various prior research studies. I found it reasonable to include certain material from my earlier publications. For example, Chapter 5 is devoted to solutions of particular industrial problems and implementation of scientific results.

Anatoly D. Alexeev
Donetsk, Ukraine

Acknowledgments

I gratefully acknowledge all the contributors who participated in writing this book. They, like me, endeavored to contribute their best to the theory and applications of the physics of coal and mining processes. Most of them are researchers at the Institute for Physics of Mining Processes of the National Academy of Sciences of Ukraine. They are Professor A. Y. Granovskii (Introduction, Sections 1.1 and 1.2); Candidate V. V. Slusarev (Section 1.3); Dr. E. V. Ulyanova (Section 1.4 and Chapter 5); Candidate A. K. Kirillov (Section 1.5); Professor E. P. Feldman and Candidate V. A. Vasilkovskii (Chapter 2); Dr. V. N. Revva (Chapter 4); Dr. G. P. Starikov (Sections 4.4 and 4.5); and Professor A. E. Filippov (Section 5.4).

I am also thankful to readers for their patience in covering this complex material and for their comments and advice. I hope this volume will be useful for scientists, technicians, and engineers, and also for students, especially those pursuing mining careers.

Author



Anatoly Dmitriyevich Alexeev is the leading earth scientist in Ukraine. Dr. Alexeev has combined a career in physics, chemistry, and engineering with teaching, research, and writing more than 300 publications, 14 monographs, and 50 patents. He developed the theory of gas absorption and emission in porous media and an applied approach to extreme states of rocks and rock massifs.

Dr. Alexeev's areas of interest in basic and applied research include the physics of rocks and mining processes, radiophysics, extreme states of solids, and physico-chemical mechanics. He studied the effects of surficants on stress states of rocks and implemented surfagents to prevent outbursts in coal mines. He also applied nuclear magnetic resonance (NMR) to studies of methane–coal systems and developed new methods and technologies for predicting mine outbursts.

Dr. Alexeev is a corresponding member of the National Academy of Sciences of Ukraine, a member of the Academy of Mining Sciences of Ukraine, and the Russian Academy of Natural Sciences. He graduated from Donetsk Polytechnical Institute in 1963 and joined the institute as an assistant professor. He was named head of the laboratory in 1967. In 1992, Dr. Alexeev became the division director of the Donetsk Physical and Technical Institute of the National Academy of Sciences of Ukraine. He was named the director of the National Academy's Institute for Physics of Mining Processes in 2001. In recognition of his accomplishments, Dr. Alexeev was awarded the State Prize of Ukraine (1996), the A.A. Skotchinsky prize (1990), and the I. Puluy prize (2001). He was designated an Honored Miner of Ukraine (1996) and received several President's medals in all three classes for "Valiant Labour," "Miner's Glory," and "Miner's Valour."

Contents

Foreword	vii
Preface.....	ix
Acknowledgments	xi
Author	xiii
1 Coal Structure	1
1.1 Genesis of Coal Substance	2
1.2 Elemental Composition of Coals.....	5
1.3 Structure of Organic Mass.....	8
1.4 X-Ray Studies.....	17
1.4.1 Literature Review.....	17
1.4.2 Structural Peculiarities of Coal–Methane System	31
1.4.3 New Approach to Analyzing Coal via Scattering X-Ray Investigation.....	37
1.4.3.1 Materials and Methods	41
1.4.3.2 Results and Discussion.....	42
1.4.4 Conclusions.....	53
1.5 Porosity.....	53
1.5.1 General Characteristics	54
1.5.2 Neutron Scattering	59
1.5.3 Fractality	63
1.5.4 Closed Porosity of Donbass Coals.....	69
1.6 Conclusions.....	78
References	80
2 Equilibrium Phase States and Mass Transfer in Coal–Methane Systems	87
2.1 Equilibrium and Dynamics of Mass Exchange between Sorbed and Free Methane.....	87
2.1.1 Gaseous State of Methane in System of Opened and Closed Pores	87
2.1.2 Solid Solution of Methane in Coal: Absorption and Adsorption.....	90
2.1.3 Diffusion of Methane from Coal Lumps into Filtration Volume: Efficient Diffusion Coefficient.....	93

2.2	Joint Flow of Filtration and Diffusion Processes in Coal Massifs.....	94
2.2.1	Double-Time Models of Mass Transfer: Fast and Slow Methane.....	94
2.2.2	Methane Escaping from Coal into Closed Volume: Role of Backpressure	98
2.2.3	Methane Flow from Coal Seam into Worked-Out Space.....	104
2.3	Methane Accumulation in Dangerous Coal Lump Regions	107
2.3.1	Time for Formation of Highly Explosive Methane–Air Mixture.....	107
2.3.2	Thermodynamic Gibbs Potential for Gas–Coal Massif: Prognosis for Localization of Coal Burst Sections of Seam	111
2.4	Investigation of Phase State and Desorption Mechanisms of Methane in Coal.....	114
2.4.1	Methane Phase States in Coal.....	115
2.4.2	Kinetics and Mechanisms of Methane Desorption from Coal	126
2.4.3	Transformation of Methane Desorption Mechanism: Three Stages of Desorption	140
2.5	Conclusions.....	143
	References	144
3	Nuclear Magnetic Resonance Studies of Coal and Rocks.....	147
3.1	Experimental Techniques	147
3.1.1	High Resolution Spectrometers.....	147
3.1.2	Wide Line Spectrometers.....	148
3.1.3	High Pressure Technique	151
3.2	Coal Structure Research.....	157
3.2.1	Determining Structural Components of Coals through ^1H NMR Data	157
3.2.2	Application of ^{13}C NMR for Analyzing Coal Structures.....	158
3.2.3	Research of Donets Basin Coals.....	160
3.3	Phase States of Water and Methane in Coal.....	161
3.3.1	Water–Coal Adsorption.....	163
3.3.2	Adsorption by Impulse NMR.....	170
3.3.3	Water in Rocks.....	182
3.3.4	Methane in Coal.....	187
3.4	Phase State of Binding in Rocks.....	195
3.4.1	Polymer Compositions in Coals	195
3.4.2	Binding in Rocks.....	200
3.5	Conclusions.....	209
	References	210

4 Behaviors of Rocks and Coals in Volumetric Fields of	
Compressive Stresses.....	215
4.1 Experimental Technique.....	215
4.1.1 Literature Review.....	216
4.1.2 True Triaxial Compression Unit	220
4.2 Strength Properties of Rocks Treated by Different Binders	226
4.2.1 Experimental Methods and Estimates of Strengthening.....	227
4.2.2 Width of Fissure Openings	229
4.2.3 Moisture of Rocks under Strengthening.....	230
4.2.4 Temperature of Surroundings	232
4.2.5 Conclusions.....	233
4.3 Influence of Loading Method and Loading History on Volumetric Strength.....	234
4.3.1 Loading Method	234
4.3.2 Loading History	237
4.3.3 Conclusions.....	240
4.4 Coal Destruction	240
4.4.1 Mechanism of Coal Destruction.....	241
4.4.2 Filtration Properties.....	249
4.4.3 Changes of Fissured and Porous Structures.....	252
4.5 Limit State	254
4.6 Post-Limit State.....	261
4.6.1 Essence of Problem	262
4.6.2 Post-Limit Deformation under True Triaxial Compression	264
4.7 Conclusions.....	272
References	273
5 Genesis of Natural Gases, Methane Extraction, and Coal	
Mining Safety	277
5.1 Genesis of Gases in Coal-Bearing Series	277
5.1.1 Methane Isotopic Analysis: Literature Review	278
5.1.2 Methane Isotopic Analysis: Experiment and Discussion.....	279
5.1.3 Mossbauer Spectroscopy	282
5.1.4 Stoichiometry of Reaction.....	285
5.1.5 Conclusions.....	287
5.2 Dependence of Outburst Proneness on Mineral Inclusions	288
5.2.1 Experiments and Discussion.....	288
5.2.2 Conclusions.....	292
5.3 Electromagnetic Method of Seam Degassing	292
5.3.1 Electric Dipole	301
5.3.2 Magnetic Dipole.....	302
5.3.3 Conclusions.....	303

5.4	Physics of Fissured Porous Coal Structure Transformation under Influence of Unloading Wave	303
5.4.1	Influence of Gas Content on Stability of Coal– Gas System	304
5.4.2	Modeling of Porous Medium	308
5.4.3	Movement of Wave of Unloading.....	310
5.4.4	Transformation of Pores into Fissures	316
5.5	Classification of Gas-Dynamic Phenomenon Type.....	318
5.5.1	Criteria of GDP	320
5.5.2	Parameters and Technology of Method	324
5.6	Predicting Coal Seam and Sandstone Outburst Danger.....	327
5.6.1	Outburst Dangers of Coal Seams	327
5.6.1.1	Criteria for Outburst Danger.....	327
5.6.1.2	Criteria for Outburst Estimation.....	327
5.6.1.3	Grounding and Testing of Outburst Prediction Method at Openings of Steep Seams.....	332
5.6.2	Rock and Gas Outbursts	335
5.7	Safe Extraction of Coal	341
5.7.1	Outburst Control Measures.....	341
5.7.2	Safe Load on Working Face	349
5.8	Conclusions.....	351
	References	351
	Index	359

1

Coal Structure

Fossil coal is a “living witness” of prehistoric times (from the Carboniferous to Jurassic), when the Earth was covered with impenetrable jungles, and equisetums, lycopodiums, and ferns thrived. Due to seismic cataclysms, the jungles were first buried under water and later under various rock layers. That started the transformation of wood material into coal—a process known as metamorphism. Meanwhile, the world’s oceans witnessed a similar process—the transformation of plankton into petroleum.

Petroleum is a natural accumulation of hydrocarbons. Its deposits occur in sedimentary rocks of various ages. Crude oil is an insoluble, dark brown, oily liquid with a density of 0.75 to 0.95 g/cm³. It contains 83 to 87% carbon, 11 to 14% hydrogen, and minor amounts of nitrogen, oxygen, and sulfur. Cyclic hydrocarbons are dominant in some oil grades and chain polymers are dominant in others.

The chemistry of petroleum formation has not yet been fully elucidated, but most likely the source material was provided by life remains in shallow sea basins. Rapid development of primitive algae resulted in a rapid evolution of animal life. In view of the enormous reproductive rapidity of protozoa under favorable conditions, it is not surprising that great amounts of their remains accumulated at the bottoms of bodies of water. In the absence of air, the remains slowly decomposed in near-bottom waters and were gradually covered with clay and sand, steadily transforming into petroleum over millions of years.

Two competitive energy carriers emerged: coal and petroleum. They differ in form (one is solid, the other liquid). This difference is certainly important. Petroleum is easily transported via pipelines; coal must be repeatedly trans-shipped from origin to user. Furthermore, petroleum recovery is far less complicated. It requires only wells instead of mines. However, the crucial difference between these energy carriers that determines their recovery and use is caloric efficiency (approximately 8 kcal/g for coal and 11 kcal/g for petroleum). These values correspond to the transformation levels of the electron shells (0.4 and 0.6 eV/atom, respectively).

The second important feature is the amount of the world’s reserves of these traditional energy resources. The estimates indicate more than 1.5×10^9 tons for coal; 0.17×10^9 m³ for petroleum, and 1.72×10^{11} m³ for gas. With respect to the amount and total energy content, petroleum ranks second to coal by an order of magnitude. As energy demands increase by approximately 3% per year, energy consumption in 2025 will amount to 2.28×10^7 tons of equivalent fuel. If industry as the main energy consumer continues to grow at this rate,

the world resources of coal, petroleum, and gas will be exhausted in approximately 100 years. Note, however, that this holds for explored reserves (and also recoverable ones with regard to coal). What geologists may discover in the future remains unknown although estimates are still in favor of coal. Gas energy in the Ukraine amounts to 41% (21% world average). Additional sources are coal and petroleum (19% each), and uranium (17%); other sources constitute 4%. Manufacture of a commercial product with a cost of \$1 requires 0.9 kg of equivalent fuel or 2.5 times the world average.

The specified values of 8 to 11 kcal/g for coal and petroleum, respectively, are minor in comparison to the caloric efficiency of a uranium fission reaction that produces as much as 10^4 times the energy. Thus, many countries prefer nuclear fuel to coal and petroleum as sources of chemical raw materials. Russia, for example, satisfies 16% of its needs through nuclear energy because its nationwide cost per equivalent unit is 13 to 15% less than the average. Nuclear fuel is virtually the most feasible energy source to replace limited and nonrenewable reserves of petroleum and coal. This problem still remains open. After sufficient thermonuclear energy sources are developed, coal and petroleum as energy carriers will be regarded as insignificant, and pass to the domain of chemists. Then perhaps the reversion to Mendeleev's idea of underground coal gasification will become possible.

Comparing coal with petroleum, we have passed over one general question: why do coal and petroleum liberate heat during combustion? More precisely, why exactly do they burn? The answer is simple. The C–C and C–H bonds that characterize hydrocarbons possess less energy (81 kcal/g-atom) than the C=O bond (85 kcal/g-atom) after combustion. This benefit of 4 kcal/g-atom does ensure caloric efficiency. Furthermore, combustion involves surmounting a certain energy barrier—somewhat low for petroleum and higher for coal. Under natural conditions, spontaneous ignition may occur due to the sulfides in beds that decrease this barrier.

What predominant problems does any physicist encounter when beginning studies of coal? The first step is to establish the general physical properties and create a certain model of its structure. Then one may proceed to analyze its behavior during interactions with various surrounding materials (gases, liquids, rocks, etc.) in different stress fields.

1.1 Genesis of Coal Substance

During carbonization, the content of the basic coal-forming elements in the organic matter of coals changes considerably.* Coal properties are predeter-

* A very complete systematic survey of coal typology, physicochemical properties, and structure can be found in a monograph by D.W. Van Krevelen [22]. We also employed studies of coal constitution to solve physical problems encountered in coal recovery.

mined by the manner of accumulation, surrounding conditions of sedimentation, and plant material required to form coal from peat. The first stage of carbonization is biochemical. Peat is the less metamorphosed product of the transformed plant bodies. It is a heterogeneous, porous (up to 70%) mixture consisting of decayed parts of dry land and marsh land vegetation that underwent different stages of transformation. It contains 55 to 65% carbon, 5 to 7% hydrogen, 30 to 40% oxygen, and 1 or 2% nitrogen and it approximates the composition of timber (50% carbon, 6% hydrogen, 44% oxygen, and 0.1 to 0.5% nitrogen on average). The composition of the most recent deposits of peat closely resembles the composition of timber. Under close examination, peat may reveal bands characteristic of brown and even black coals.

Because of limited oxygen presence, diagenesis occurs on peat surfaces. Decomposition of lignin provokes synthesis of humic acids that undergo carbonization and generate vitrinite. During the biochemical stage of carbon formation, decayed vegetation initially liberates colloids (heterogenic unstructured systems). Coal coagulation structures are not strong originally but their strength increases as water leaves the solidifying colloid and the coal substance consolidates.

Formation of the condensed coal structure is complete at the point of transition from the biochemical to the geochemical stage. Because of the loss of functional groups and simultaneous compaction of the aromatic ring in the crystallization lattice (both events typical for coal transformation during carbonization), black coal, in contrast to peat or brown coal, is harder, always black, less moist, and more compact. The formation of a condensed coal structure arises from increasing pressure and temperature and dehydration and compaction of colloid substances in the absence of oxygen.

A variety of geological and genetic factors led to formation of coals with different physical, chemical, and technological properties. Within a single coal basin, it is possible to categorize coals according to their maturity. On average, black coals of the Donets Basin constitute 75 to 80% vitrinite groups, 4 to 12% fusainite groups with large amounts of condensed aromatic fragments, and 6 to 12% liptinite groups, the latter having the longest aliphatic chains and providing aliphatic structural parts for the coal material.

Carbonization results from the influence of certain physical factors affecting the entire coal-bearing stratum and embraces all the beds. At the stage of diagenesis, an average of vitrinite reflection (R_0) amounts to 0.4%. During catagenesis, its value dramatically increases, reaching 2.6 to 5.6% at metagenesis (of anthracites). It follows that petrographic composition and metamorphism degree are two independent variables that determine coal properties. As the extent of carbonization rises, the ratio of chemical elements alters and the carbon contents in the aromatic ring networks and quantity of aromatic rings increase. The lattices of their clusters become more rigid and the coal eventually acquires the properties of a solid. The microhardness of vitrinite in brown coal-anthracite (B–A) series, for instance, becomes five times as great. This change is most apparent at lean coal-anthracite (T–A) stage [1].

Coal is a product of decayed organic materials from earlier geological ages. Carbonization progress depends on external conditions and the duration of their influence and results in multiple metamorphism products such as coals (brown, black, anthracite), sapropelites, pyroschists, and petroleum. Anthracites and graphites are considered the most perfect structures among coals and represent completion of the metamorphic line. Representative anthracites reveal properties unusual for bituminous coals (enhanced electrical conduction, for instance). It is believed that under certain conditions anthracite can pass through the intermediate stages to transform into graphite. In this case graphite concludes the succession from peat to lignite to bituminous coal to anthracite.

In its free state, carbon exists in three modifications (1) cubic lattice (diamond) (2) hexagonal graphite, and (3) hexagonal lonsdaleite extracted from meteorites or synthesized. A black diamond with graphite lattice was found first on the Moon, and later on Earth. Amorphous carbon does not occur in natural conditions. Graphite is composed of linked carbon networks (layered lattices) that account for the softness and flakiness observed while drawing with a graphite pencil. Each atom of carbon is bonded to four others. Distances to three of them are similar (0.142 nm), whereas the fourth atom is more distant (0.335 nm) and contributes a weaker bond. This feature manifests itself in the easy splitting of graphite into separate layers.

Attracting force between the layers is small, enabling the layers to glide over one another. Graphite peculiarities may result from a short-term (epoch—no more than 1,000 years) but powerful impact of an intrusive thermal field (up to 1,000°C) on already formed coal materials. In response to such an effect, graphite and vitrinite assume fine-grained structures, the spacing between carbon lattice planes decreases, carbon content increases, and ordering of the whole structure is enhanced. Graphite preserves the cellular structures of coal-forming plants [2].

In nature, solids have well defined macromolecular structures that may be regarded as molecules whose atoms are covalently bonded.

Comparatively few substances in a solid state can generate atom lattices. One example of such a lattice is the diamond—one of the free forms of carbon. Each atom of carbon forms four equal bonds with four adjacent carbon atoms to create an enormous, very durable, and consolidated macromolecular structure at the expense of common electron couples by strong covalent bonds that enable high hardness and high boiling and melting temperatures. Diamonds naturally originated from a combination of hard-to-reproduce conditions that liberated free carbon. While natural diamonds formed along with the Earth's crust by crystallization of carbon dissolved in melted magma, artificial diamonds are made under specific conditions within kimberlite pipe, and subjected to high pressures and temperatures for a long period; carbonization terminates at the stage of graphite. Contemporary physics laboratories succeeded in synthesizing fullerenes and nanotubes not yet found in nature.

Despite the experimental evidence on artificial carbonization, the significance of geological time must be regarded as a long-term impact on any factor (temperature, for instance) that may produce different results from organic material transformation under different timing conditions.

1.2 Elemental Composition of Coals

It may seem unusual to open a study of the physics of mining processes with a chapter related to the chemical composition of coals. This paradox, however, is absolutely natural because all the macroscopic properties of coal are dependent on microscopic ones that are in turn conditioned by atomic properties; thus the boundary between physics and chemistry disappears.

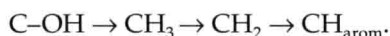
The basic coal components are carbon, hydrogen, and oxygen. Carbonization is associated with regular and specific alterations of the amounts of these elements. The many variations among carbon compounds account for its peculiar properties, the most significant of which is ability to form strong atomic bonds. Due to the strength of bonding, molecules containing chains of carbon atoms are adequately stable under ordinary conditions, whereas molecules with similar chains of other elements are not nearly so strong.

The energy of the C–C bond (83 kcal/mole) is sufficient to provide stability for chains of virtually any length. x-ray examinations have shown that the carbon atoms in such compounds with linear structures are arranged not along a line, but along a zigzag. This results from carbon's four valences directed in a certain way toward one another; their relative position corresponds to lines drawn from the center to vertices of a tetrahedron. Carbon in organic compounds may exist in an aromatic state. This is defined as a special type of atom bonding into plane cycles (closed chains) in which all the atoms in a cycle participate in formation of a uniform electron system of bonding. Benzene is the simplest aromatic compound that forms a structural unit that determines the properties of all aromatic compounds.

In studies of coals via various physical and chemical techniques, it was found that an average of condensed aromatic cycles per structural unit ranges (subject to metamorphic grade) from 4 to 10 cycles with 80% of total carbon in cyclic components [3]. The high molecular structures of coals that include aromatic, hydroaromatic, heterocyclic and aliphatic components, and functional groups, are generally recognized. However, no uniform view indicates exactly how these fragments are connected, how the structural units are built, and how they communicate with the spatial system (see Section 1.3).

Organic matter of coal may be generally described as a mixture of condensed molecules whose C=C double bonds are represented only by aromatic bonds, and some carbon, hydrogen, oxygen, nitrogen, sulfur, and

other heteroatoms form side aliphatic groups at the condensed aromatic nuclei. The oxygen-containing components in the aliphatic segments of the organic coal substance allow connections of the organic and non-organic contents. Various types of interaction are possible, for example, adsorption (electrostatic adsorption, hydrogen bonding, chemisorption), complexing (coordinate bonding), and formation of metal–organic compounds via the inclusion of heteroatoms or homopolar bonding. Essentially, the relative carbon content in the metamorphic line increases according to the pattern:



For coals with $V^{\text{daf}} = 28\%$, $\text{C-OH} = 1.8\%$; $\text{CH}_3 = 7.6\%$; $\text{CH}_2 = 12.0\%$; $\text{CH}_{\text{arom}} = 20.8\%$; $\text{C}_{\text{arom}} - \text{C}_{\text{arom}} = 57.8\%$.

With increasing grades of metamorphism, concentrations of oxygen-containing groups decline, structural fragments become more homogeneous and ordered, and transformation of various components of the coal substance (those having undeveloped bonds and considerable oxygen and aliphatic components) proceeds into a three-dimensional homogeneous structure with a large poly-condensed system containing minimal amounts of hydrogen and heteroatoms.

As the degree of carbonization increases, reactions remove oxygen and hydrogen from coal as CO , CO_2 , CH_4 , and H_2O . At the middle stage of metamorphism, loss of hydrogen in such coals increases with rising oxygen presence, helping enhance the flexibility of macromolecules in the coal substance on the one hand and forming strong bonds between the fragments of the structure at the expense of the oxygen-containing functional groups on the other hand. During the formation of anthracites, with pressure as the predominant metamorphic factor, nitrogen, sulfur, and other heteroatoms undergo redistribution from the condensed systems of the molecular structure to the periphery. Classification of coals is traditionally based on grades of metamorphism (see Table 1.1).

Oxidation leads to self-heating and spontaneous combustion of coals. Oxidation initially involves aliphatic hydrogen and carbon; aromatic ones

TABLE 1.1

Rank Classification of Coals

Description	V	G	F	C	LB	L	A
Yield of volatiles V (%)	37	35–37	28–35	18–28	14–22	8–18	8
Carbon content (%)	78	81–85	85–88	88–89	90	91–94	94–98
Hydrogen content (%)	5.3	5.2	5.0	4.7	4.3	3.9	3.2

Source: Kizilshtein L.Y. 2006. *Geochemistry and Thermochemistry of Coals*. Rostov University Press, Rostov on Don.

V = volatile. G = gaseous. F = fat. C = coking. LB = lean baking. L = lean. A = anthracite.