

# Structure and Reactivity of Coal

Ke-Chang Xie

# Structure and Reactivity of Coal

A Survey of Selected Chinese Coals

 Springer

Ke-Chang Xie  
Taiyuan University of Technology  
Taiyuan  
China

and

Tsinghua University  
Beijing  
China

ISBN 978-3-662-47336-8      ISBN 978-3-662-47337-5 (eBook)  
DOI 10.1007/978-3-662-47337-5

Library of Congress Control Number: 2015941120

Springer Heidelberg New York Dordrecht London  
© Springer-Verlag Berlin Heidelberg 2015

This work is subject to copyright. All rights are reserved by the Publisher, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilms or in any other physical way, and transmission or information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed.

The use of general descriptive names, registered names, trademarks, service marks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

The publisher, the authors and the editors are safe to assume that the advice and information in this book are believed to be true and accurate at the date of publication. Neither the publisher nor the authors or the editors give a warranty, express or implied, with respect to the material contained herein or for any errors or omissions that may have been made.

Printed on acid-free paper

Springer-Verlag GmbH Berlin Heidelberg is part of Springer Science+Business Media  
([www.springer.com](http://www.springer.com))

# Contents

<b>1 Geological Characteristics of Coal</b> . . . . .	1
1.1 Coal Formation . . . . .	1
1.1.1 Components of Coal Formation . . . . .	2
1.1.2 Formation of Humic Coal . . . . .	5
1.2 Classification of Coal . . . . .	10
1.2.1 Peat . . . . .	10
1.2.2 Lignite . . . . .	11
1.2.3 Bituminous Coal . . . . .	11
1.2.4 Anthracite . . . . .	11
1.2.5 Technical Classification of Coal in China . . . . .	12
1.2.6 Coal Resources and Distribution in China . . . . .	13
1.3 Coal Macerals . . . . .	14
1.3.1 Coal Lithotype . . . . .	15
1.3.2 Organic Macerals of Coal . . . . .	16
1.3.3 Inorganic Macerals . . . . .	21
1.3.4 Separation and Enrichment of Coal Macerals . . . . .	22
1.3.5 Quantitative Analysis of Coal Macerals . . . . .	23
1.3.6 Chemical Composition of Coal Macerals . . . . .	24
1.3.7 Relationship Between Coal Type and Rank . . . . .	26
References . . . . .	27
<b>2 Physical Characteristics of Coal</b> . . . . .	29
2.1 Physical Properties of Coal . . . . .	29
2.1.1 Mechanical Properties of Coal . . . . .	29
2.1.2 Thermal Properties of Coal . . . . .	33
2.1.3 Optical Properties of Coal . . . . .	34
2.1.4 Electrical and Magnetic Properties of Coal . . . . .	37
2.1.5 Surface Properties of Coal . . . . .	38
2.1.6 Coal Models . . . . .	42

2.2	Physical Methods for Coal Structure Characterization . . . . .	43
2.2.1	Infrared Spectroscopy . . . . .	43
2.2.2	Nuclear Magnetic Resonance Spectroscopy . . . . .	49
2.2.3	X-ray Diffraction . . . . .	52
2.2.4	Small-Angle X-ray Scattering . . . . .	54
2.2.5	Electron Microscopy . . . . .	54
2.2.6	Surface Methods . . . . .	55
2.3	Statistical Constitution Analysis . . . . .	60
2.3.1	Coal Structural Parameters . . . . .	60
2.3.2	Principle of Statistical Constitution Analysis . . . . .	62
	References . . . . .	64
<b>3</b>	<b>Chemical Characteristics of Coal . . . . .</b>	<b>67</b>
3.1	Chemical Properties . . . . .	67
3.1.1	Moisture in Coal . . . . .	67
3.1.2	Mineral Matter and Ash in Coal . . . . .	69
3.1.3	Volatile Matter and Fixed Carbon in Coal. . . . .	71
3.1.4	Elemental Composition. . . . .	73
3.1.5	Calorific Value . . . . .	78
3.1.6	Basis of Coal Analysis Indicators. . . . .	82
3.1.7	Functional Groups in Coal . . . . .	84
3.2	Chemical Methods for Coal Structure Determination. . . . .	88
3.2.1	Solvent Extraction . . . . .	89
3.2.2	Computational Chemistry . . . . .	93
3.3	Case Study of Coal Chemical Structural Analysis. . . . .	97
3.3.1	Macromolecular Network Structure of Pingshuo Coal. . . . .	97
3.3.2	Micromolecules Structure of Pingshuo Coal . . . . .	108
3.3.3	Summary . . . . .	115
	References . . . . .	117
<b>4</b>	<b>Coal Pyrolysis Reactions. . . . .</b>	<b>119</b>
4.1	Introduction to Coal Pyrolysis . . . . .	119
4.1.1	Pyrolysis Processes . . . . .	120
4.1.2	Chemical Reactions of Coal During Pyrolysis . . . . .	125
4.1.3	Kinetics of Coal Pyrolysis. . . . .	128
4.2	Study of Coal Pyrolysis . . . . .	133
4.2.1	Study of Coal Pyrolysis by PyGC Technique . . . . .	133
4.2.2	Study of Coal Pyrolysis by Py-FTIR Techniques . . . . .	138
4.2.3	Study of Coal Pyrolysis by Thermogravimetry. . . . .	143
4.3	Pyrolysis Simulation Applied to Coalification Case Study . . . . .	152
4.3.1	Main Factors Affecting Simulation Experiments. . . . .	154
4.3.2	Simulation Study of Coalification . . . . .	157

4.4	Structure–Reactivity Relationships in Coal Pyrolysis . . . . .	168
4.4.1	Application of Pyrolysis Methods in Study of Coal Structure–Reactivity Relationships . . . . .	168
4.4.2	Application of Solvent Extraction in Research on Coal Structure and Reactivity . . . . .	171
4.4.3	Model Compounds in Studies of Coal Structure and Reactivity . . . . .	173
4.4.4	Models for Pyrolysis Reactivity . . . . .	173
	References . . . . .	178
<b>5</b>	<b>Coal Gasification . . . . .</b>	<b>181</b>
5.1	Introduction to Coal Gasification . . . . .	181
5.1.1	Gasification Reactivity Research . . . . .	182
5.1.2	Gasification Reaction Mechanisms . . . . .	183
5.1.3	Catalytic Gasification Mechanisms . . . . .	185
5.2	Thermogravimetric Behavior of Coal and Its Macerals Gasification . . . . .	187
5.2.1	Non-catalytic Gasification of Coal . . . . .	188
5.2.2	Catalytic Gasification of Coal . . . . .	195
5.3	Compensation Effects in Gasification Reactions . . . . .	203
5.3.1	Compensation Effects and Coke Gasification Dynamic Parameters . . . . .	204
5.3.2	Theoretical Analysis of Compensation Effect . . . . .	206
5.4	Studies of C–O Complexes Over Coal Surface with TPD . . . . .	213
5.4.1	Pretreatment of Samples . . . . .	214
5.4.2	TPD Study of C–O Complexes . . . . .	215
5.4.3	Analysis of CO <sub>2</sub> Gasification of Cokes Based on TPD Results . . . . .	220
5.5	Structure–Reactivity Relationships in Coal Gasification . . . . .	220
5.5.1	Factors Affecting Gasification Reactivity . . . . .	220
5.5.2	Relationship Between Coke Crystal Structure and Gasification Reactivity . . . . .	229
5.5.3	Relationship Between Coke Surface Properties and Gasification Reactivity . . . . .	231
	References . . . . .	240
<b>6</b>	<b>Coal Depolymerization and Liquefaction . . . . .</b>	<b>243</b>
6.1	Introduction to Coal Depolymerization and Liquefaction . . . . .	243
6.1.1	Coal Depolymerization and Liquefaction Methods . . . . .	244
6.1.2	Low-Temperature Coal Liquefaction Depolymerization Reactions . . . . .	245

6.2	Studies of Depolymerization and Liquefaction of Shenfu Coal . . .	250
6.2.1	Base-Catalyzed Methanol–Coal Depolymerization . . . . .	251
6.2.2	Extraction and Separation of Products in Base-Catalyzed Methanol–Coal Reaction. . . . .	252
6.2.3	Distribution of Extraction Products of Shenfu Coal Depolymerization Under Different Reaction Conditions . . . . .	253
6.2.4	Fourier-Transform (FT) IR Analysis of Extracted Fractions from Shenfu Coal Depolymerization. . . . .	253
6.2.5	GC-MS Analysis of Extraction Fractions from Shenfu Coal Depolymerization. . . . .	260
6.2.6	Reactivity of Shenfu Coal in Methanol–Alkali Systems . . . . .	263
	References . . . . .	268
<b>7</b>	<b>Coal Combustion . . . . .</b>	<b>269</b>
7.1	Introduction to Coal Combustion . . . . .	269
7.1.1	Combustion Reactions . . . . .	270
7.1.2	Pore Models of Coal Combustion . . . . .	277
7.1.3	Studies of Changes in Surface State During Combustion of Four Coal Samples. . . . .	279
7.2	Kinetics of Coal Combustion. . . . .	289
7.2.1	Studies of Kinetics of Coal Combustion Using Temperature-Programmed Thermogravimetric Analysis (TGA). . . . .	289
7.2.2	Coal Combustion Kinetics Under Fixed-Bed Conditions . . . . .	292
7.2.3	Isothermal TG Studies of Combustion Kinetics . . . . .	296
7.2.4	Fractal Analysis of Combustion Kinetics. . . . .	297
	References . . . . .	303
<b>8</b>	<b>Coal Swelling . . . . .</b>	<b>305</b>
8.1	Introduction to Coal Swelling . . . . .	305
8.1.1	Measurement and Calculation of Swelling Ratio . . . . .	306
8.1.2	Model of Coal Physical Structure and Swelling Process . . . . .	309
8.1.3	Factors Affecting Swelling Ratio . . . . .	311
8.1.4	Swelling During Pyrolysis. . . . .	315
8.2	Study of Swelling Behaviors of Coals. . . . .	318
8.2.1	Degree of Swelling . . . . .	318
8.2.2	Swelling Mechanism . . . . .	321
8.2.3	Changes in Coal Caused by Swelling. . . . .	329
	References . . . . .	334

<b>9 Coal Plasma Reactions</b> . . . . .	337
9.1 Introduction to Plasma Coal Pyrolysis. . . . .	337
9.1.1 Coal Pyrolysis and Other Reactions in Arc Plasma. . . . .	338
9.1.2 Applications of Plasma Technology in Coal-Based Chemical Industry . . . . .	346
9.2 Thermodynamic Equilibrium of Chemical Reactions in Multiphase Carbon–Hydrogen–Argon–Oxygen Systems. . . . .	350
9.2.1 Calculation Methods. . . . .	351
9.2.2 Thermodynamic Data and Equilibria. . . . .	355
9.3 Acetylene Production Experiments Involving Coal Pyrolysis in a Plasma . . . . .	362
9.3.1 Experimental Devices . . . . .	362
9.3.2 Conversion Calculations . . . . .	365
9.3.3 Coal Pyrolysis in Arc Plasma . . . . .	366
9.4 Simulation of Coal Devolatilization in Plasma . . . . .	384
9.4.1 Devolatilization Model . . . . .	384
9.4.2 Chemical Percolation Devolatilization (CPD) Model. . . . .	386
9.4.3 Applications of CPD Model . . . . .	392
9.5 Coke Formation Mechanism in Arc Plasma . . . . .	400
9.5.1 Factors Affecting Coking . . . . .	401
9.5.2 Properties of Coking Material . . . . .	406
References . . . . .	411