Physical Chemistry in Action

Emilia Wołowiec-Korecka

Carburising and Nitriding of Iron Alloys

Springer

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ISSN 2197-4349 ISSN 2197-4357 (electronic)
Physical Chemistry in Action
ISBN 978-3-031-59861-6 ISBN 978-3-031-59862-3 (eBook)
https://doi.org/10.1007/978-3-031-59862-3

This Springer imprint is published by the registered company Springer Nature Switzerland AG
The registered company address is: Gewerbestrasse 11, 6330 Cham, Switzerland

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I dedicate this book to my beloved husband, Maciej.

Preface

The actual conditions in which science operates are directing the research towards utilitarianism. Almost every application for research project funding these days includes a question about the advisability of the planned research and the viability of its implementation. An important question, therefore, is: how do we analyse and value the development trends of thermo-chemical treatment in order to correctly identify those that are prospective? Meanwhile, it is difficult to assess contemporary development trends, influenced by the uneven balance of the vast scientific literature and the scarcity of sources concerning practical applications. The aim of this book is to present a structured, albeit simplified, picture of modern thermo-chemical treatment to answer questions about the causes, relationships, and trends in this area of science. Cognition and explanation serve to understand the reality, and understanding is the ideal state: it allows you to optimise activities in the future without a widely conceived waste of time and resources. Tracing the development and attempting to bring together the scattered knowledge into a coherent study seems a worthwhile endeavour, although it is clear that it is impossible to provide a comprehensive and exhaustive description in a single volume.

Global thermal treatment and thermo-chemical treatment (TCT) remain fragmented, and the research and development efforts necessary to innovate the industry are only being pursued in certain segments, despite the fact that expectations as to the quality and precision in product manufacture are steadily increasing and the correct selection of treatment parameters and maximising their impact are becoming increasingly important. A key challenge of modern TCT is to achieve high repeatability and uniformity of manufactured products at high volume and mass scale.[1] Additional trends are set by the modern organisation of industrial production—observed especially in the automotive industry—where the concept of management by quality is becoming the standard for production management in companies. This new way of thinking and approaching management problems, using statistical process control,

[1] The global heat treating market size was valued at USD 100.73 billion in 2021 and is expected to expand at a compound annual growth rate of 3.4% from 2022 to 2030 (Grand View Research, 2021).

is the basis for an organisation to operate in a way where the quality of the manufactured product is the guiding element and at the same time the link between all spheres of activity.

The uncompromising market economics of the twenty-first century make the contemporary utilitarian development of thermo-chemical treatment possible in two ways: (1) by offering quality at a level unachievable for competitors or (2) by reducing manufacturing costs without losing quality. Both trends are evident in the current development of thermo-chemical treatment and are often linked in some way. However, finding their new areas of applicability is combined with developing knowledge of these processes. Today, many gaps in the contemporary state of knowledge are being filled based on high-performance computer calculations, which have become part of the canon of the modern scientific research workshop. Computational models and simulations contribute to both reducing manufacturing costs and improving production quality. For this reason, the following chapters discuss the contemporary development of thermo-chemical treatments against the background of the parallel development of computational capabilities, pointing out references in the literature, available scientific research and known practical applications.

The book is divided into seven chapters, discussing quenching, carburising and nitriding individually, although the issues sometimes overlap. Chapter 1 provides an introduction to the work and identifies the importance of materials engineering against the background of contemporary societal needs. Chapter 2 discusses thermo-chemical treatment and its development over the centuries. The modern challenges for thermo-chemical treatment globally are presented next. Chapters 3–5 present the three main development trends: reduction of thermal deformation in mass and high-volume production, TCT modelling and a broadly perceived reduction of the costs of conducting the treatment. These are identified in the literature at the dawn of the twenty-first century as important and necessary to be addressed quickly. This is the Author's subjective choice, as the list of important issues is much longer (this topic is discussed at length in Chap. 2). Chapter 6 describes the importance and contribution of computational methods to the development of thermo-chemical treatment. All the issues discussed and the challenges of the future are succinctly summarised in Chap. 7, which concludes the work.

This study provides a literature review of the development trends of modern thermo-chemical treatment and, in this respect, fills a gap in the literature on this topic. Due to the review nature of the work, it can serve as supplementary literature in subjects covering surface engineering for students of materials engineering and mechanical engineering.

Łódź, Poland
January 2024

Emilia Wołowiec-Korecka

Declarations

Competing Interests The author was an R&D manager of a research grant from the National Centre for Research and Development of Poland as part of project no. POIR.04.01.04-00-0087/15 entitled: “Equipment for high performance and precise heat treatment with a quenching deformation reduction system for direct application in downstream production chains of mechanical gearing and bearings”. The research results presented on some figures and tables in Chaps. 3 and 4 were financed from this grant (Figs. 3.2, 4.2, 4.3, 4.4, 4.5, 4.6 and Table 3.7).

Ethics Approval None of the studies presented in this book were conducted on patients or animals.

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Acknowledgements

This book would not have been created in its current form without the participation and support of others. Many scholars and friends helped me during the various stages of working on this book when I encountered various difficulties. It is not possible for me to list all the people who deserve it, but I would like to mention the most important ones:

I would like to thank Prof. Piotr Kula, who in many ways shaped my view of materials engineering, including the belief that there must be utilitarian aspects to scientific work.

I would like to thank Prof. Jerzy Michalski for his careful reading of the first version of the book and his accurate comments and suggestions, which helped to give it a much better final shape.

I would like to thank Prof. Leszek Klimek for answering my many questions about materials engineering and for being an inexhaustible source of literature.

I would like to thank Prof. Leszek A. Dobrzański for his kindness and for motivating me to "stay at the course of the work".

I would like to thank my husband Maciej for his constant love and belief that nothing is impossible. Our discussions on low-pressure single-piece flow carburising have laid the foundations for the subject matter of this work.

I extend my thanks to three great practitioners of thermal and thermo-chemical treatment: Daniel Herring—for generously sharing his scientific and industrial knowledge and donating a large amount of literature of his own authorship, Prof. Richard Sisson—for working together as part of the CHTE team and providing an opportunity to observe what it is like to work in a scientific-industrial consortium in a US setting, and Dr. D. Scott McKenzie—for the opportunity to view global activities in thermal and thermo-chemical treatment from the perspective of ASM International. Daniel, Richard and Scott have been my benevolent guides in the world of global commercialisation of thermal and thermo-chemical treatment.

I would like to thank two women of science: Dr. Marzena Kraszewska and Prof. Anna Dobrzańska-Danikiewicz, the embodiments of uncompromising determination in the pursuit of scientific excellence, from whose attitude I was inspired.

I would like to thank my supervisors, Prof. Łukasz Kaczmarek and Prof. Jacek Sawicki, for creating favourable conditions for working on the book, and my friends, Dr. Aleksandra Jaszczak and Anna Gnatkowska, for their continued support.

During the work on Chap. 6, dedicated to computational techniques, I was accompanied by the memory of Dr. Jerzy Dobrodziej, Eng. I know that he would have taken up the challenge of writing this work before me if he had not passed away prematurely.

When writing the book, I used the original texts wherever possible. This was possible, in particular, owing to the Jagiellonian Digital Library, the Main Library of the AGH University of Science and Technology and the Podlasie and Lower Silesia Digital Libraries. I would like to thank the Staff of these institutions, whose work in digitising Polish old prints has enabled me to travel less during pandemic.

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Symbols and Acronyms

β_C	Carbon transport coefficient
β_N	Nitrogen transport coefficient
γ'	Layer of γ' nitrides
ε	Layer of ε nitrides
ε	Strain
ε^e	Elastic strain
ε^p	Plastic strain
ε^{tr}	Transformation plasticity strain
ε^{th}	Thermal strain
ε^{df}	Diffusion induced strain of carbon/nitrogen
ϕ	Volume fraction of the transformed phase
ρ	Density
σ	Stress
σ^y	Yield stress
ω	Dissociation rate
c	Heat capacity
d	Distance
h	Heat transfer coefficient
k	Speed reaction factor
m	Mass
m_{N_2}	Nitrogen availability
p	Pressure
t	Duration, time
w	Weight fraction
x	Mole fraction
C	Carbon concentration
C_P	Carbon potential
CD_{Eff}	Effective case depth
CD_{Tot}	Total case depth
D	Diffusion coefficient
D_C	Carbon diffusion coefficient

D_N	Nitrogen diffusion coefficient
F	Flow
Fe_α	Iron allotrope (ferrite)
Fe_γ	Iron allotrope (martensite)
J	Flux
J_Q	Heat flux
K	Heat conduction coefficient
L	Latent heat due to phase transformation
M_f	Final temperature of martensite transformation
M_s	Initial temperature of martensite transformation
N	Nitrogen concentration
N_P	Nitrogen potential
R	Boltzmann constant
S	Surface
T	Temperature
V	Volume
σ	Standard deviation for population
r	Range
s	Standard deviation for sample
$\overline{x}$	Mean value for sample
C_p	Process parameter scatter coefficient
C_pk	Process parameter distribution position coefficient
V	Coefficient of variation
ADALINE	ADAptive LINear Element
AI	Artificial Intelligence
BEM	Boundary Element Method
CFD	Computational Fluid Dynamics simulation
CPS	Cyber-Physical System
CVD	Chemical Vapour Deposition method
DL	Deep Learning
DM	Data Mining methods
FDM	Finite Difference Method
FEM	Finite Element Method
FVM	Finite Volume Method
HPGQ	High-Pressure Gas Quenching
IoT	Internet of Things
KDD	Knowledge Discovery in Databases
k-NN	k-Nearest Neighbours method
LPC	Low-Pressure Carburizing
LPN	Low-Pressure Nitriding
LSM	Least Squares Method
ML	Machine Learning
MLP	Multi-Layer Perceptron neural network
NN	Neural Network
PVD	Physical Vapour Deposition method

RBF	Radial Basis Function neural network
SPC	Statistical Process Control
SVM	Support Vector Method

Chapter 1
Introduction

You cannot fight against the future.

Wiliam Gladstone, 1809–1898

Our civilisation is changing and developing, and with it the expectations of the societies of different countries are changing. The social transformations over the centuries are so significant that, in sociological and economic sciences, the successive stages in the development of societies have been given names of their own, in the likeness of industrial revolutions [1]. The term Society 1.0 is used to describe a prehistoric stage in which people lived in small communities, providing food for themselves by hunting or gathering edible plants. This was followed by the agrarian period (Society 2.0), in which people farmed the land, cultivating a grain culture and becoming an agricultural society. This period saw the emergence of statehood and money as a means of exchanging resources. The amount of land owned became a measure of wealth. The turn of the seventeenth and eighteenth centuries brought further social transformations, linked to the Industrial Revolution (Society 3.0), concentrating multitudes of workers in newly established urban agglomerations. The invention of the steam engine and the introduction of electrification ensured that production lines operated around the clock; man's daily routine therefore changed radically to suit shift work in factories. The computerisation and robotisation of production lines in the second half of the twentieth century has again transformed the way society lived, making it an information society (Society 4.0). Data processing has become as important as matter processing—information gathering and exchange have become values in themselves, providing unlimited access to knowledge for people all over the globe. Today, data collected in the cloud and processed by artificial intelligence algorithms shape our daily lives, for example, by providing automatic translation of texts on the Internet, navigation on a mobile phone, searching for information on Google, or

E. Wołowiec-Korecka, *Carburising and Nitriding of Iron Alloys*, Physical Chemistry in Action, https://doi.org/10.1007/978-3-031-59862-3_1

even controlling the home washing machine, fridge and oven. Moving forward, in 2016, the first country, Japan, signalled the need for another transformation improving the social life, postulating that this is only possible through the effective use of large-scale data (Society 5.0).[1]

The Japanese now define the term Society 5.0 as a human-centred model of human relations (human-centric society). This model uses economic progress to solve social problems through a system and technology that strongly integrates cyberspace with physical (real) space. Thus, we are talking about a society characterised by a higher level of integration (interpenetration) of the two realities—the digital reality and the genuine reality—facilitating the embedding of cyberspace in the real world [2, 3]. Japan was the first to propose a new model of how society should operate in response to the problems of energy shortages and foreign imports of energy, limited natural resources and an unfavourable demographic structure. An important aspect of this solution is the use of artificial intelligence methods (AI).

The concept described above—of developing the functioning of society—is also impossible without the advanced development of materials and the development of techniques for their manufacture. A parallel philosophical shift in the approach to the problem of materials and their production is needed to satisfy the signalled societal needs, as indicated by a comparative analysis of materials development in the context of societal development (Table 1.1). As will be substantiated below, in the context of the social assumptions made, there is no alternative to the development of industrial product manufacturing other than in line with the concept of Industry 4.0. The state of knowledge presented in this study also supports this thesis.

While Japan is in the vanguard of some social crises, other countries also have cause for concern. The unfavourable shape of the demographic structure is also evident in Europe, as is trouble in the energy sector. However, Europeans seem to be open to novelty in the way they function as a society just as much as they declare themselves open to using new technologies. According to a study by the Digital Poland Foundation conducted in Poland, 26% of Poles are techno-enthusiasts, 54% are techno-sceptics, 6% are picky technology users and only 14% are technology rejecters. Every year there is a growing tendency amongst Poles to settle their tax obligations via the Internet, to use electronic banking or to use e-providence [6]. It seems, therefore, that the vision of Society 5.0 is already meeting with a favourable response.

Material 4.0 and Industry 4.0

The term Industry 4.0 is derived from D. Bell's concept of industrial revolutions (Table 1.2). The first industrial revolution was named for the process of technological, economic, social and cultural changes initiated in the eighteenth century in England and Scotland, which saw the transition of production from craftsmanship

[1] Society 5.0—a human-oriented society in which economic progress proposing solutions to social issues is balanced by a system offering a high integration of digital and real space.

Table 1.1 Development of societies in the context of the materials engineering development [3–5]

<table>
<tr><th colspan="2">State of social development</th><th colspan="2">State of materials engineering</th></tr>
<tr><td>Society 1.0</td><td>Hunters-gatherers-societies (from 70 000 years BC.); basic social unit: group; trade exchange—barter; no privacy; division of labour by gender</td><td rowspan="3">Selection by trial and error: chemical composition of materials, process conditions of manufacture, range of applications</td><td rowspan="3">Material 1.0</td></tr>
<tr><td>Society 2.0</td><td>Agricultural society (from 8 000 years BC.); statehood; basis of exchange: money; land as a basis of wealth; functional division of labour</td></tr>
<tr><td rowspan="2">Society 3.0</td><td rowspan="2">Industrial society (from XVII/XVIII w.); concentration of population in cities on a massive scale; rigid, complex division of labour</td></tr>
<tr><td rowspan="2">Idea and laboratory works: characterisation, laboratory prototyping, testing and validation, pilot production, life cycle assessment</td><td rowspan="2">Material 2.0</td></tr>
<tr><td rowspan="3">Society 4.0</td><td rowspan="3">Information society (from 1955, USA); most important work with and on information; middle class; networks of formal and informal links</td></tr>
<tr><td>Modelling of a hypothetical material with assumed functionality: characterisation, laboratory prototyping, testing and validation, pilot production, life cycle assessment</td><td>Material 3.0</td></tr>
<tr><td rowspan="2">Big data type of data on materials fabrication and properties; computational materials science using artificial intelligence methods (AI), machine learning algorithms (ML), multiscale modelling; virtual materials synthesis and characterisation, prototyping, testing and validation; life cycle assessment</td><td rowspan="2">Material 4.0</td></tr>
<tr><td>Society 5.0</td><td>Society of imagination (from the 10th of the twenty-first century); integration of real-world cyberspace on the basis of technology; global community's pursuit of prosperity; smart manufacturing; digital transformation in which informationalisation is dominant</td></tr>
</table>