

Heat and Mass Transfer

Series Editors

Dieter Mewes, Universität Hannover, Hannover, Germany

Franz Mayinger, München, Germany

This book series publishes monographs and professional books in all fields of heat and mass transfer, presenting the interrelationships between scientific foundations, experimental techniques, model-based analysis of results and their transfer to technological applications. The authors are all leading experts in their fields.

Heat and Mass Transfer addresses professionals and researchers, students and teachers alike. It aims to provide both basic knowledge and practical solutions, while also fostering discussion and drawing attention to the synergies that are essential to start new research projects.

More information about this series at <http://www.springer.com/series/4247>

Vladimir Danilov · Roman Gaydukov ·
Vadim Kretov

Mathematical Modeling of Emission in Small-Size Cathode

Vladimir Danilov
National Research University
Higher School of Economics
Moscow, Russia

Roman Gaydukov
National Research University
Higher School of Economics
Moscow, Russia

Vadim Kretov
National Research University
Higher School of Economics
Moscow, Russia

ISSN 1860-4846

Heat and Mass Transfer

ISBN 978-981-15-0194-4

<https://doi.org/10.1007/978-981-15-0195-1>

ISSN 1860-4854 (electronic)

ISBN 978-981-15-0195-1 (eBook)

© Springer Nature Singapore Pte Ltd. 2020

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, expressed or implied, with respect to the material contained herein or for any errors or omissions that may have been made. The publisher remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

This Springer imprint is published by the registered company Springer Nature Singapore Pte Ltd. The registered company address is: 152 Beach Road, #21-01/04 Gateway East, Singapore 189721, Singapore

Preface

The study described in this book began several years ago when Prof. M. V. Karasev acquainted the authors with two MIET (National Research University “Moscow Institute of Electronic Technology”) researchers, N. A. Dyuzhev and M. A. Makhboroda who reported at the seminar that the mathematical modeling of electron emission from small-size cathodes has not yet been investigated full enough. The main problem in this study is the modeling of heat transfer with possible cathode melting.

The global (this term is explained in the book below) description of the heat transfer with melting taken into account can be obtained using the phase-field system, i.e., in the framework of the contemporary generalization of Stefan-type problems.

The phase-field model has already been studied during approximately 15 years in the mathematical literature but, as it turned out, the specialists in the field of electronics knew nearly nothing about it. The result of this model adoption is discussed in the book proposed to the reader.

It should be noted that the electron tunneling process was studied (mainly, from the physical viewpoint) in detail for semiconductors and metals in G. Fursey’s book.¹ But the numerical modeling described in that book gave a very high temperature of the cathode but without taking the possibility of melting into account.

The proposed monograph mainly deals with mathematical modeling, namely it describes the mathematical model of heat transfer in a silicon cathode of small (nano) dimensions with the possibility of partial melting taken into account. This is a mathematically very difficult problem, and the properties of the solution of the phase-field system underlying our study have not yet been described completely. We present only well-known analytic results, but the basic idea in this book is the following one.

Instead of a pure mathematical approach, we apply an approach based on the understanding of the solution structure and computer simulation. The understanding of the solution structure is based on the construction of asymptotic solutions and an

¹G. Fursey “Field Emission in Vacuum Microelectronics”, Springer (2005).

analysis of their properties. The further comparison of the results of numerical experiments with the asymptotic solutions allows us to determine the process behavior and its characteristics.

Further, note that not all details of physical processes in the cathode (especially in the case of appearance of the liquid phase) have been described in the literature. Therefore, in numerical experiments, we made several additional assumptions. Moreover, in this book, we briefly consider some information given in the physical literature which (from our viewpoint) explains the properties of the mathematical model.

All physical parameters contained in our model can be found in the physical literature, i.e., in different reference books. The only exception is the expression describing the Nottingham effect. All physical constants in this expression are known, but the formula itself is obtained on the basis of tunneling through the potential barrier from half-plane to space. Thus, the actual geometry of the cathode is not taken into account in this formula. Usually, in problems of such a type, the cathode geometry is taken into account by using the so-called form-factor. We follow this way choosing a multiplier in the expression for the heat flow from the emitter surface. This multiplier is the only “adjusting” parameter in our problem and can easily be determined experimentally by comparing the theoretical value of the emission flow density (from the plane surface of the emitter) with the actual emission current observed in experiments.

The book is organized as follows. In Chap. 1, we describe the history of discovering the electron emission phenomenon and its types. We also present the mathematical statement of the problem of the field emission from semiconductor cathodes of small dimensions.

In Chap. 2, we briefly discuss some information from the solid-state physics, in particular, formulas for specific conductivity, thermoelectric height, and the Thompson coefficient for semiconductors. We also mathematically describe the tunneling process through the potential barrier on the cathode–vacuum interface, write a formula for the field emission current density in the case of metals, and describe its specific features in the case of field emission from semiconductor cathodes. At the end of the second chapter, we describe the Fowler–Nordheim theory and the Nottingham effect in the case of field emission from metals.

In Chap. 3, we discuss the phase-field model and the basic properties of its solutions. We also present formulas for asymptotic solutions of the phase-field system in the simplest case and in some special cases.

In Chap. 4, we present formulas for the numerical solution of the system of phase-field equations and an algorithm for solving the problem numerically (including its realization by contemporary multiprocessor systems and hybrid systems based on graphic accelerators) and discuss the results of numerical experiments.

Preface to the English Edition

In addition to the Preface to the Russian edition, we would like to make some remarks. The book deals with the physical problem—electron emission from a small-size cathode.

We initially intended to solve the problem of phase transition concerning the field emission of electrons from a small-size cathode. Obviously, the small size of the cathode and a relatively strong electric current density through it could result in melting of the cathode core. Thus, it was necessary to solve the Stefan problem taking into account the large curvature of the boundary between phases (the latter follows from the small size of the cathode).

If one begins to think about numerical calculations of the Stefan problem solution, then he immediately comes to the idea of adaptive mesh or something like this. A significant difference between geometric sizes (extremely small near the top of the cathode and relatively large near the bottom) results in additional troubles. Thus, to obtain the global solution of the phase-field system approximating the solution of the original problem seemed to be the most simple way to solve the problem.

We would like to stress that for the research work described in the book, we have to use relatively contemporary mathematical tools, especially the last results of the theory of generalized functions.

The most important point here is the construction of the definition of generalized solution to the phase-field system; see Sects. 3.4 and 4.6. As was discovered, the initial stage of melting required a special construction of liquid-phase nucleus for its description, where we actively used the concepts of mushy region and interaction of nonlinear waves; see Sect. 3.5.

And finally, we propose to use visualizations simultaneously with pure mathematical considerations to investigate the mathematical model; see Sect. 3.5.

The mathematical background is not the main part of this book, but, by our opinion, it would be better to learn about it before one starts his own investigations in the field described here.

For this edition, we checked and corrected many misprints and added some comments through out the text.

Moscow, Russia
July 2019

Vladimir Danilov
Roman Gaydukov
Vadim Kretov

Acknowledgements

The authors express their deep gratitude to Professor of Department of Applied Mathematics HSE University (National Research University Higher School of Economics), M. V. Karasev, for the useful discussions and comments when the manuscript was prepared in the Russian language.

The authors thank Rector of MTUCI A. S. Adzhemov (Moscow Technical University of Communication and Informatics) for the help in publishing the monograph (in Russian).

The authors also thank Professor of Department of Applied Mathematics HSE University, V. M. Chetverikov, for the useful remarks.

The study of V. G. Danilov, R. K. Gaydukov, and V. I. Kretov was implemented in the framework of the Basic Research Program at the National Research University Higher School of Economics (HSE University).

Contents

1	Introduction	1
1.1	Brief History of the Electron Emission Discovery	1
1.2	Types of Electron Emission	2
1.3	Statement of the Problem	4
1.4	Mathematical Statement of the Problem. Heat Transfer Model	7
	References	9
2	Physical Basis for Field Emission	11
2.1	Energy-Band Theory and Fermi Level	11
2.2	Conductivity of Semiconductors	16
2.2.1	Electron and Hole Concentration	17
2.2.2	Effective Mass	20
2.2.3	Electron and Hole Mobilities	21
2.2.4	Temperature-Dependence of Conductivity in Silicon	22
2.3	Thermoelectricity	22
2.4	Emission Current Density and Nottingham Effect	24
2.4.1	Support Function in Metals	26
2.4.2	Electron Tunneling Through the Potential Barrier	27
2.4.3	Formula for the Barrier Transparency Factor in the Case of Field Emission Cathode	39
2.4.4	Emission Current Density in Metals	43
2.4.5	Specific Characteristics of Field Emission from a Semiconductor Cathode	43
2.4.6	Approximation of the Formula for the Emission Current Density	46
2.4.7	Nottingham Effect	48
2.4.8	Optimal Values of Approximation Parameters	52
2.4.9	Dependence of the Inversion Temperature on the External Electric Field Strength	54
	References	56

3	Mathematical Model	59
3.1	Phase Field System and its Use in Heat Transfer Modeling	59
3.2	Phase Field System as Regularization of Limiting Problems with Free Boundary	64
3.3	Asymptotic Solution of the Phase Field System and Modified Stefan Problem	70
3.3.1	Construction of an Asymptotic Solution	73
3.3.2	Examples	82
3.4	Weak Solution of the Phase Field System and the Melting Zone Model	84
3.4.1	Weak Solutions and Rankine–Hugoniot-Type Conditions	88
3.4.2	Solutions of “Wave Train” Type and the Corresponding Limiting Problem	97
3.5	Derivation of the Solution of the Limit Stefan–Gibbs–Thomson Problem from a Numerical Solution of the Phase Field System . . .	113
3.6	Generation and Coalescence of Dissipative Waves	121
	References	128
4	Numerical Simulation and its Results	131
4.1	Nanocathode Model	131
4.2	Calculation of the Current Density Inside the Cathode	135
4.3	Calculation of the Emission Current Density and Modeling of the Nottingham Effect	137
4.4	Difference Scheme	138
4.4.1	Difference Scheme for the Equation for the Potential	141
4.4.2	Difference Scheme for the Equation for the Order Function	143
4.4.3	Difference Scheme for the Heat Equation	145
4.4.4	Stability of the Difference Scheme	147
4.4.5	One More Version of the Difference Scheme	151
4.4.6	Choice of Steps of the Difference Scheme	154
4.5	Algorithm for Solving the Difference Equations and Possible Versions of its Parallelization	155
4.6	Some Remarks About the Calculation of the Electric Potential . . .	159
4.7	Results of Numerical Experiments	164
4.7.1	Nonmonotone Behavior of Free Boundaries	165
4.7.2	Results of Modeling with Physical Parameters Corresponding to Experimental Data	166
4.8	Formation of Melting and Crystallization Nuclei in the Model . . .	170
4.9	Conclusion	187
	References	193