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Mathematical modeling of heat transfer with adjustment for melting in the conical cathode

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Relevance of the dissertation

The electron emission from a solid body looks like an interesting phenomenon that has different practical applications. In particular, the electron beam devices, electronic microscopes and other devices work due to electron emission.

This study explores emission from conical field emission small size cathodes. Such cathodes are used in FEM microscopy and electronic lithography. The research of creating displays based on small size FEM cathodes was declared some time ago. The cathodes are made of different materials: wolfram, silicon, other metals and semiconductors. We consider cathodes made of silicon but our model can also be applied for cathodes made of different materials, namely, of metals and semiconductors.

A significant and still incompletely investigated problem is the degradation of FEM cathodes during the emission process. This degradation is caused by the strong heating of the cathodes due to electric current flows through them. The heating leads to partial melting of the cathode and changes its geometry. That is why the modeling of heat distribution in the cathode, formation of liquid phase domains, and motion of free interfaces between different phases is important for detection of operational conditions of the devices with FEM cathodes.

Besides the heating due to the current, there is another temperature effect that influences the temperature, i.e., the Nottingham effect that consists in cooling the cathode spike during emission. This effect is also taken into account in the current study.

The degree of development for the research problem

The model of heat distribution in the cathode was considered in [8] but without the possibility of the cathode melting taken into account. Besides, in [8], the Fauler–Nordheim approximation is used to calculate the emission current density value, but this approximation cannot be applied at high temperatures which may be attained during the field emission process. In the current study, the specific features of this emission process are taken into account.

Formulas for the emission current density in semiconductor devices are most precisely considered in [9], [10] and [11]. It is worth to note that the field emission theory for semiconductors was developed already in the 1950—1960s and was mostly represented in R. Stratton studies, see, for example, [11]. However, not all predictions of Stratton's theory were confirmed [10]. That is why, this dissertation is based on the more recent results mainly obtained in [10].

The mathematical model of heat transfer is based on the studies of Cadginalp [12, 13, 14], where the regularization of the Stefan–Gibbs–Thomson problem was proposed as a phase field system. This regularization was rigorously proved in [15] and [16]. In the last study by V.G. Danilov, G.A. Omelyanov, E.V. Radkevich, the definition of generic solution that allows passing to the limit from the phase field system to the Stefan–Gibbs–Thomson problem was proposed. Besides, the Stefan problem is precisely reviewed in monograph [17] (and many of other Meyrmanov studies, that are referred to in that monograph). In Meyrmanov's works, the properties of generic solution of the Stefan problem are explored in detail and an example of nonclassical solution (mushy region) is constructerd. The phase field system was applied in A.M. Lashin work to model the pure metal crystallization (see [18]). In the monograph [19], the exact solution of Stefan problem and the solution representation in the form of integrals and series were obtained and numerical methods for solving the problem were considered. Several questions related to numerical solution of the heat equation including the Stefan problem were considered in detail in [20]. One more work related to the Stefan problem is [21].

The mathematical model in the form of phase field system is used in the dissertation. To pass to the limit from the phase field system to the Stefan–Gibbs–

Thomson problem, an asymptotic estimate is proved. This estimate includes a small parameter of the phase field system and constants from the Gibbs–Thomson condition. This estimate ensures the correctness of passing to the limit if these constants are small. And besides, the estimate is obtained for both the exact solution of phase field system and the approximate numerical solution constructed by the finite difference method.

Objectives and goals of the research

The main goal of the dissertation research is to create the heat transfer model in the conical field emission cathode with the possibility of melting and the Nottingham effect taken into account and to perform a numerical analysis of the heat profile in the emitter operation.

To reach the assigned target, the following problems are solved:

1. Construction of the model of heat transfer in conical field emission cathode based on the phase field system.
2. Justification of the orrectness of passing to the limit from phase field system to the Stefan–Gibbs–Thomson system.
3. Construction of the algorithm for calculating the emission current density.
4. Modification of the phase field system for taking the liquid phase domain formation into account.
5. Software implementation for performing the numerical modeling and analyzing its result.

Scientific novelty of the work

The new mathematical model is presented in this study. This model describes the heat transfer and melting in a small size conical semiconductor field emission cathode. This model includes the heat equation with right-hand side modeling the Joul heating, the Allen-Cahn equation describing the dynamics of solid/liquid phase interface with order function, and the electric field potential equation. The calculation results obtained by this model are presented and analyzed. And a new method for modeling the origination of the liquid phase domain in the cathode is proposed[1].

The reliability of the obtained results

The results presented in the dissertation are obtained by rigorous mathematical methods such as asymptotic methods, methods for studying nonlinear equations of mathematical physics, and methods for numerically solving the differential equations with finite differences. All new assertions formulated in the dissertation are rigorously proved. The solutions of obtained equations are illustrated with their numerical solutions b y using the algorithm based on finite differences satisfying the maximum principle. The calculation algorithms and the software package based on these algorithms are tested on the well-known exact solutions of the equations composing the mathematical model.

Basic results presented to be defended

1. A mathematical model based on the phase field system for analytic and numerical analysis of the heat transfer and processes of free boundary motion in the small size conical cathode is constructed. The model takes the Nottingham effect and cooling through the underlying surface into account.

2. Passing to the limit from the finite difference scheme of phase field system to the Stefan—Gibbs–Thomson problem is studied. It is shown that the constructed mathematical model is the regularization of the physical problem of the heat transfer with a free boundary.

[1] The method for adding the liquid phase nuclei differs from the method described in [22]

3. According to the constructed mathematical model an authentic algorithm for computing the emission current density is developed which can replace the well-known Fauler–Nordheim approximation.

4. A modification of the constructed model is proposed for modeling the origination of the liquid phase domain in the cathode.

5. A software package for implementing the proposed model is created. A numerical analysis of the temperature dependence on the cathode physical parameters is performed using this package. Also the liquid domain origination is analyzed, and the main parameters that influence the temperature distribution are detected. The results obtained from numeric experiments are consistent with the experimental data [23].

Description of the research methodology

To solve the given problem, theoretical methods for investigating the nonlinear equations of mathematical physics and methods for numerically solving the differential equations with implicit nonfinite difference schemes are used. To justify the applicability of the phase field system, we used elements of generalized functions theory. Finite difference schemes were solved by using the method of alternating directions. Numerical calculations were performed by using the developed software package written in the C++ language. The open source libraries Qt, Qwt and muParser were used.

Theoretical and practical significance

The practical and theoretical significance of the dissertation study is determined by the possibility of analyzing the heat profile of field emission cathodes for designing devices with such cathodes. Although the modeling does not allow one to avoid experimental work for optimal adjustment of the cathode parameters, it can significantly reduce the amount of this work. Also it can be further developed to improve its accuracy. The model can be used, for example, to investigate the heat profile of the cathodes operating in electronic microscope cantilevers. The results of this study can be applied in the research in the area of heat transfer processes and field emission.

Approbation of work

The main results were reported at the following scientific-technological conference and seminars:

1. Scientific-Technological Conference of MIEM Students, Postgraduate Students, and Young Scientists, 2011.

2. The World Congress on Engineering and Technology (CET2012), Beijing, China, 2012.

3. The 4th International Conference of Young Mathematicians on Differential Equations and Their Applications Dedicated to Ya.V. Lopatinskii, Donetsk National University, Donetsk, Ukraine, 2012.

4. Scientific-Technological Conference of MIEM Students, Postgraduate Students, and Young Scientists, 2014.

5. International Conference on Computer Simulation in Physics and Beyond (CSP2015), HSE, 2015.

6. Scientific-Methodological Seminar NIVTs MGU, 2016.

7. Scientific Seminar “Asymptotic Methods in Mathematical Physics” under the guidance of Doctor of Phys.-Math. Sci., Professor S.Yu. Dobrokhotov, IPM, RAS, 2017.

8. Scientific Seminar “Asymptotic Methods in Mathematical Physics” under the guidance of Doctor of Phys.-Math. Sci., Professor S.Yu. Dobrokhotov, IPM, RAS, 2018.

The report theses were published in [24, 25, 26].

Personal contribution of the author to the development of the problem

The author actively participated in the process of constructing the model and in analyzing the results of modeling. The author also developed the software complex for the modeling and carries out a series of numerical experiments for testing the program and analyzing the modeling results. All results included in the dissertation

General research conclusions

1. A mathematical model for analytical and numerical analysis of the heat transfer and the process of motion of free boundaries in a small size conical cathode based on the phase field system. The boundary conditions in the model are used to take into account the Nottingham effect on the upper base of the cathode and the heat release on the lower base.

2. The passing to the limit from the difference scheme for the phase field system to the Stefan—Gibbs—Thomson problem is studied. It is shown that the constructed mathematical model is a regularization of the physical problem of heat transfer with free boundary.

3. An algorithm for calculating the emission current density is developed so as to replace the Fauler–Nordheim approximation which cannot be used in the problem considered here.

4. A modification of the constructed model is proposed which is indented to model the liquid phase domain origination in the cathode.

5. A software complex is developed for realizing this model. The certificate of official registration of the computer program is obtained.

6. The constructed model and the program are used to perform a numerical analysis of the temperature dependence on different physical parameters of the cathode and of the liquid phase domain origination. In this case, the physical parameters are consistent with the known experimental data [23]. Several significant parameters determining the thermal regime of the cathode operation are revealed.

List of publications in the topic of the dissertation

The materials of the thesis were published in 7 printed works, 2 of them included in the Scopus citation system, 1 publication included in the list of journals recommended by HSE. One certificate of state registration for computer program is obtained. The publications contain all main results of dissertation work. In the publications with coauthors at least 50 % of results belong to the aspirant. All results presented to be defended belong to the author.

The results presented to be defended are contained in the following publications.

Articles published by the author in peer-reviewed scientific journals, included in the international abstract database and citation system Scopus:

1. Danilov V., Gaydukov R., Kretov V., Rudnev V. Modelling of Liquid Nuclei Generation for Field-Emission Silicon Nanocathode // IEEE Transactions on Electron Devices. 2014. Vol. 61. No. 12. — 1 a.sh.

2. Rudnev V., Kretov V. I., Dyuzhev N. A., Makhiboroda M. A., Churilin M. N. Investigation of the thermal degradation of the silicon field-emission cathode as a two-phase system // Russian Microelectronics. 2012. Vol. 41. No. 7. P. 387–392. — 0,6 a.sh.

Articles published by the author in the leading peer-reviewed scientific journals and publications recommended by the HSE:

3. Dyuzhev N. A., Kretov V. I., Makhiboroda M. A., Rudnev V. Yu., Churilin M. N. Investigation of the heat degradation of th silicon field-emission cathode as two-phase system // News of vuzes. Electronics. 2011. №4(90), P. 23–29. — 0,5 a.sh. (in Russian)

Articles published by the author in other publications:

4. Kretov V. I. Calculation of the electric field strength in silicon field-emission cathode // Nanostructures. Mathematical physics and modeling. 2017. Vol. 16, №1, P. 59–68. — 0,6 a.sh. (in Russian)

5. Certificate №2013661633 Russian Federation. Certificate of oficial registration of computer program. Modeling of the heat transfer in small size conical field-emission cathode. / Gaidukov R. K., Danilov V. G., Kretov V. I., Rudnev V. Yu.; legal owner Federal state autonomouse educational institute of higher professional education «National Research University «Higher School of Economics» (RU). -– Claim 25.10.2013; pub. 11.12.2013, Computer program registry. — 1 p. (in Russian)

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