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The temperature distribution simulation in the graphene sublimation growth zone on SiC substrate

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The simulation results of the temperature distribution in the growth area of graphene layers obtained by the method of thermal decomposition of the silicon carbide surface substrates in setup with induction heating are presented. The heating parametrs of the setup elements are calculated using the commercial package COMSOL Multiphysics taking into account the electrical, thermal and magnetic properties of the materials from which the growth plant elements are made. A numerical estimate of the heating inhomogeneity of silicon carbide plates over its area during the growth of graphene layers at a given temperature is given. It is shown that the lateral temperature distribution over the area of the plate has radial symmetry with decreasing values towards the center.

Keywords: graphene, silicon carbide, simulation, temperature distribution, sublimation growth.

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Introduction

Today, silicon carbide (SiC) is one of the most promising materials for semiconductor electronics. High mechanical properties, high thermal conductivity, electrical conductivity, resistance to thermal loads, radiation and unique corrosion resistance make this material the choice subject in the field of creating reliable devices for power and high-frequency microelectronics and photonics [1,2]. Traditionally commercially produced SiC wafers are used as substrates in epitaxial technologies of device structures based on wide-gap materials. Recently, they were also in demand for obtaining two-dimensional layers of graphene (GR). Epitaxial growth of GR layers is carried out by thermal decomposition of the surface of SiC wafers under conditions of high-frequency (HF) induction heating up to temperatures about 2000°C [3]. The advantage of this method over the known methods of carbon deposition from an external source lies in the fact that GR structures are formed from their own atoms of the SiC crystal lattice, which ensures their higher structural quality and, therefore, reliability in conditions of further practical applications [4]. Preliminary studies showed that the optimization of the temperature distribution in the growth zone largely determines the quality of the grown GR layers. However, the designs of modern installations with RF heating allow only local pyrometric monitoring of the temperature in the growth zone through windows specially provided in their housing. In this regard, the optimization of the processes for obtaining GR, based on numerical simulation methods, is an urgent task. Note that the simulation of the processes of high-temperature synthesis of SiC single crystals by the method of physical vapor transport (PVT), also implemented in installations with RF heating, was developed since the 1990s and already proved its high efficiency [5–9]. To date, a number of commercial software packages was developed, such as Virtual Reactor, COMSOL Multiphysics, ANSYS Fluents, and others, which allow simulation based on the specific features of the equipment used and the specified growth conditions. In the present paper, using numerical methods we solved a specific analytical problem: simulation of the temperature distribution in the growth zone of GR layers on SiC substrate.

1. Experiment

Fig. 1 presents the layout diagram of the installation for growing GR on SiC, which shows the main structural elements. The growth cell and heater were made of fine-grained dense graphite, while the thermal insulation was made of porous graphite material. The elements of the installation are heated by the induction method using a high-frequency transistor generator with operating frequency of 66 kHz. Temperature is monitored throughout the entire technological process through a viewing window located in the upper flange of the reactor. The infrared optical pyrometer „Raytek Marathon MR1S“was used to measure the temperature, the measurement error of which is $\pm 0.5\%$. Pyrometric monitoring was carried out on the surface of the growth cell.

In the course of the experiments, the time dependences of the temperature during heating of the growth cell from 1000 to 2050°C and its cooling were studied at generator power values in the range of $3-10$ kW.x It was established that in the range $1000-1700$°C at power above 6 kW, the growth cell temperature change with time is close to linear (Fig. 2, a). On the basis of the dependences obtained, the

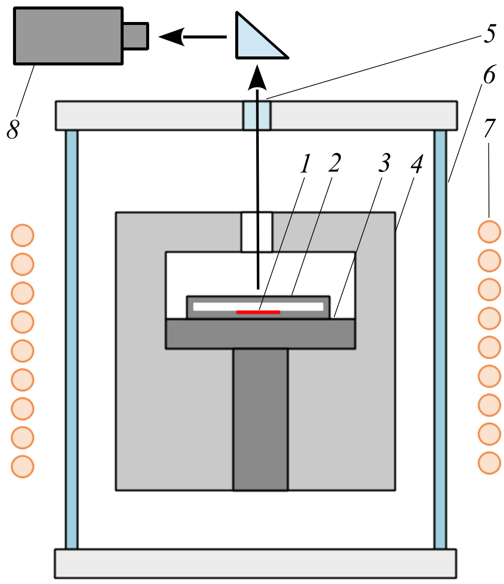

Figure 1. Schematic representation of the technological installation for growth GR, where *1* — SiC substrate, *2* — growth cell, *3* — heater, *4* — thermal insulation, *5* — pyrometric control window, *6* — quartz reactor, *7* — inductor, *8* — pyrometer.

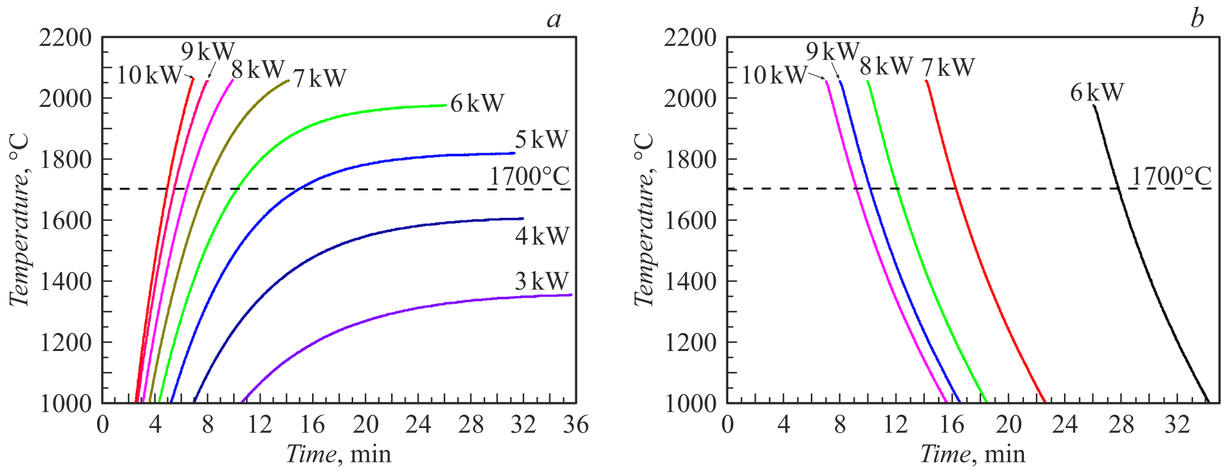

Figure 2. Temperature of the growth cell at various given values of the generator power: *a* — vs. the heating time, *b* — vs. the cooling time.

heating rates were determined at various powers. Fig. 2, *b* shows the time dependences of the temperature when the cell is cooled. As can be seen, the cell temperature vs. the cooling time in the temperature range from 2050 to 1000°C has an almost linear form. The average cell cooling rate was determined as 2.3 °C/s. Subsequently, the obtained data were used to verify the made computational model.

Numerical simulations were performed using the commercial finite element analysis package COMSOL Multiphysics. This package is an environment for simulation of physical processes of any complexity with the ability to link physical interfaces into a multiphysical system. To build a model using COMSOL Multiphysics, an axisymmetric approximation was applied, which allows obtaining a three-dimensional model of the installation based on its two-dimensional projection [10,11]. Also, all electrophysical, thermal and magnetic properties of the materials used in the installation design were taken into account. The simulation of physical processes occurring inside the growth cell was carried out using the following interfaces: „magnetic fields", „thermal conductivity", „radiation" and „convection".

2. Simulation results

Fig. 3, *a* shows a model of the installation in a heated state, obtained in the COMSOL Multiphysics program. The experimental data of temperature measurements carried out on the surface of the growth cell at different values

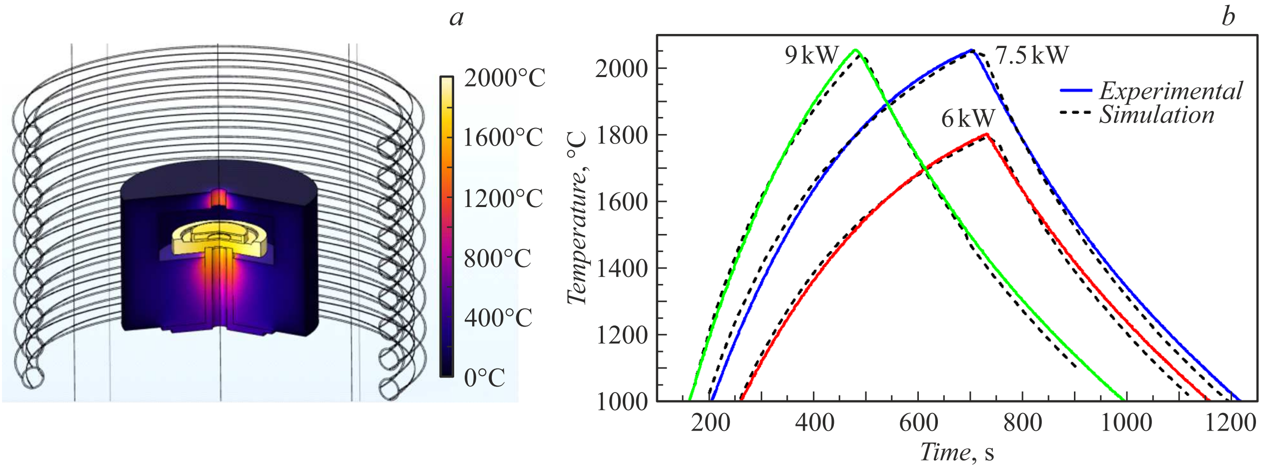

Figure 3. *a* — 3*D*-image of the installation obtained in the COMSOL Multiphysics program; *b* — experimental and calculated time dependences of the surface temperature change of the growth cell for different cycles of its heating–cooling obtained at different values of the power of the HF generator.

of the generator power and the result of simulation of the temperature change in the same region are shown in Fig. 3, *b*. It can be seen that the calculated curves are in good agreement with the experimental ones, which indicates that all the parameters of the model are set correctly, and that all interfaces are adequately linked into the multiphysics system.

Taking into account the physical properties of various materials from which the structural parts of the installation are made, the simulation of the heating temperature distribution in the growth zone, which is limited by the inner walls of the thermal insulation, was carried out. The results are shown in Fig. 4.

From the obtained results it follows that the main part of the heat is released in the area of the crucible, which indicates the effectiveness of the heat-insulating materials used and the chosen design of the growth zone. The obtained calculated results of the temperature distribution on the walls and inside the growth cell are shown in Fig. 5. As follows from Fig. 5, *a*, the lateral temperature distribution inside the cell has radial symmetry with values decreasing towards the center. In particular, at a cell surface heating temperature up to 1750°C, the change in the obtained values at a distance 1 cm from its center is 5–7°C. Fig. 5, *b* shows the curves of temperature changes on the surface of the cover and bottom of the cell. It is shown that the temperatures of the cell cover and of the cell bottom, on which the substrate is located, differ by 5–8°C.

Based on the simulation results, a quantitative assessment of the temperature scattering in the central region of the bottom of the growth cell was carried out, taking into account the geometric parameters of SiC wafers (Fig. 6). As follows from the Figure, for a square SiC wafer with a side of 5 mm, the temperature difference between its central part and the periphery is 1–2°C. For the wafer with a side of 11 mm, this difference is 7–8°C.

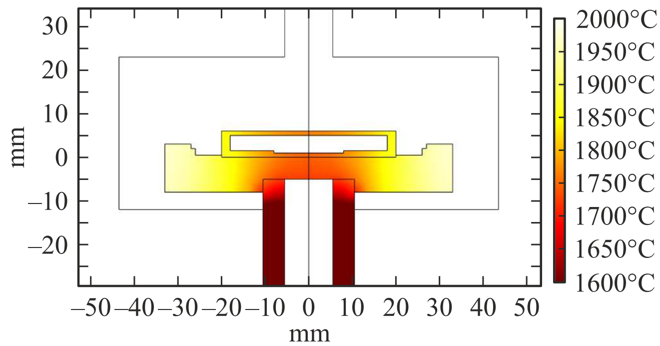

Figure 4. Temperature distribution in the growth zone.

Thus, the calculated dependences of the temperature distribution in the GR growth zone on SiC substrates were obtained for different times and powers of induction heating. The main parameters of the temperature field, which can affect the process of formation and properties of GR layers, are determined. These parameters include the difference between the temperature measured in the area of pyrometric monitoring and the actual temperature of the substrate heating, as well as the presence of temperature gradient over its area. Simulation data make it possible to correct the pyrometer readings for the specified difference and more accurately set the growth temperature of GR, as well as determine the conditions for increasing the uniformity of its distribution over the substrate area, and influence the degree of homogeneity of the properties of the obtained GR layers. The papers [12,13] present the results of studies demonstrating the high structural perfection and electrophysical properties of GR layers on SiC grown in the technological installation under consideration. The combination of previously obtained experimental results and new numerical simulation data defines new opportunities for further progress of the considered laboratory technology.

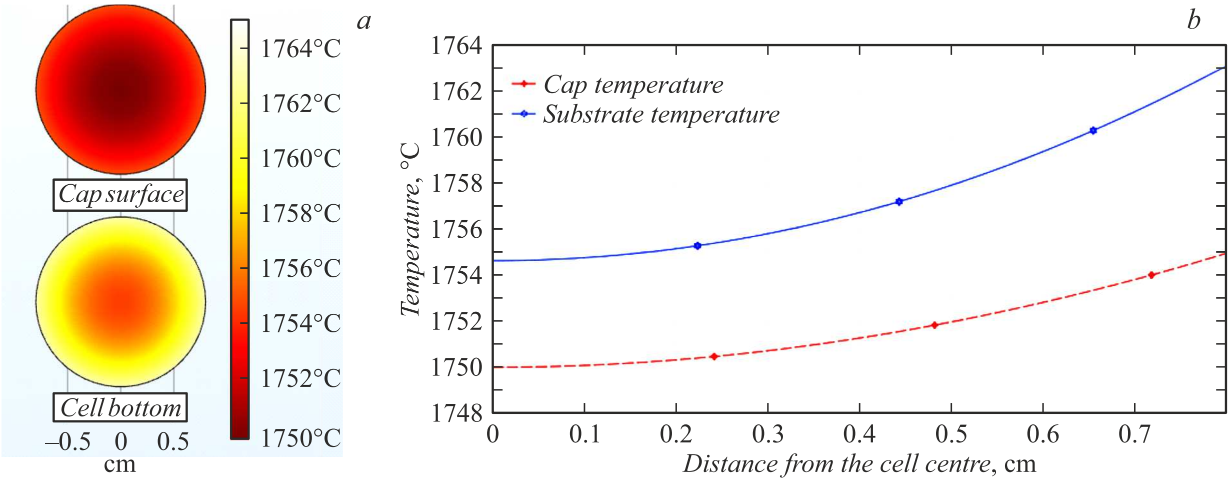

Figure 5. *a* — temperature distribution in the growth cell, *b* — graph of temperature distribution on the cover surface and on the substrate SiC surface.

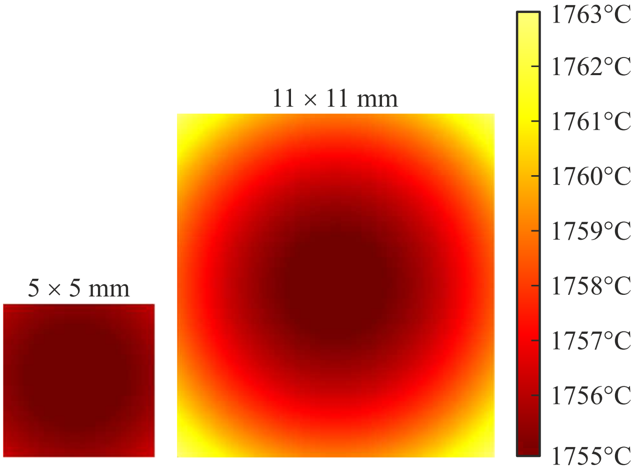

Figure 6. Temperature distribution at the bottom of the growth cell under the SiC wafer with dimensions 5 × 5 and 11 × 11 mm.

In the future, it can be expected that the use of numerical simulation in the COMSOL Multiphysics program will allow optimizing the design of the sublimation installation to solve the actual technological problem of obtaining GR based on industrially produced SiC wafers with a diameter up to 6 inches. This will ensure the transition of the developed laboratory technology for obtaining GR structures, as well as technologies for developing devices based on them to the level of industrial production.

Conclusion

The problem of multiphysics simulation of temperature distribution in the zone of epitaxial growth of GR on SiC substrates is solved. The main parameters of the temperature field distribution are determined for a specific configuration of the technological installation used for the growth of GR layers. The correspondence of experimental data and calculated parameters is demonstrated, which confirms the reliability of the model built using the COMSOL Multiphysics software package.

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Conflict of interest

The authors declare that they have no conflict of interest.

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