Computer simulation of aerosol nanoparticles focusing and deposition process for functional microstructure fabrication

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Abstract. The possibility is shown of using computer simulation to predict the size of the structures formed by the dry aerosol jet printing method. Computer modeling consisted in determining the model parameters and solving the system of equations to determine the trajectories of Ag nanoparticles of size up to 45 nm in the process of focusing and deposition through a coaxial nozzle with an outlet diameter of about 100 μm on the substrate surface located 0.5 mm away from the nozzle. As a result of the comparative analysis, a satisfactory agreement between the model and the experiment is established.

1. Introduction
Recently, printing methods have been widely developed as means for the production of inexpensive electronic circuits with the printing resolution of up to 10 μm. These methods have the prospects for the manufacture of devices such as printed antennas [1], thin-film solar cells [2], flexible displays [3], etc. Among the existing printing methods, dry aerosol jet printing (AJP) is one of the most promising methods for manufacturing functional microstructures [4]. The main advantage of dry AJP in comparison with other printing methods is the absence of the need to prepare ink to produce a flow of nanoparticles. At the same time, the dry AJP method is a relatively new and insufficiently investigated method. Thus, there is a need to develop models of dry aerosol printing processes to predict the size of the structures to be formed and to find ways to improve this technology in order to minimize the printing resolution. Therefore, in this paper, a study is presented of using computer modeling to predict the size of the structures formed by the dry aerosol printing method.

2. CFD Model
To predict the size of the structures formed by the dry aerosol printing process using computational fluid dynamics (CFD), a 2D model of the experiment on focusing and deposition of aerosol nanoparticles was constructed. The first step in constructing the experimental model was to set the geometry of the gas channel in which the focusing and deposition of aerosol nanoparticles were carried out (Fig. 1a). For detailed data on the linear dimensions and geometry of the gas channel, the data of the patent were used [5]. For the given geometry, the parameters of the dry aerosol printing process were specified. Those parameters were: the aerosol carrier gas flow rate $Q_a$, the sheath gas flow rate $Q_{sh}$, the outlet diameter of the nozzle $D_n$, the distance from the nozzle to the substrate $S$. In the experiment, argon was used for both the carrier gas $Q_a$ and the sheath gas $Q_{sh}$. The carrier gas flow rate $Q_a$ was set to 140 sccm. The sheath flow rate $Q_{sh}$ was varied from 90 sccm to 190 sccm in steps of 20 sccm. The distance from the nozzle to the substrate $S$ was set to 0.5 mm. To simplify the modeling process, and to reduce the time required for a single simulation, the entire modeling process was separated into two stages. At the first stage, the gas velocity field $\vec{u}$ in the nozzle and beyond the outlet
was computed. The velocity field was computed on the assumption that the concentration of nanoparticles does not affect the general character of the gas flow. To find the velocity field in the nozzle and outside it by the finite element method, the following system of equations was solved:

Navier–Stokes momentum equation for compressible fluid [6], [7]:

$$\frac{\partial (\rho \vec{u})}{\partial t} + \text{div}(\rho \vec{u} \otimes \vec{u}) + \vec{v} p = \rho \vec{F} + \text{div} \left( \left( \vec{v} \otimes \vec{u} \right) + \left( \vec{v} \otimes \vec{u} \right)^T - \frac{2}{3} I \text{div} \vec{u} \right)$$

(1)

Continuity equation and equation of state for perfect gas:

$$\frac{\partial \rho}{\partial t} + \text{div} \rho \vec{u} = 0; \quad p = \rho RT$$

(2)

where \( \rho \) is the medium density, \( p \) is the pressure, \( \vec{u} \) is the medium velocity, \( \vec{F} \) is external force mass density, \( \mu \) is dynamic viscosity, \( R \) is the universal gas constant, \( T \) is the temperature.

At the second stage of modeling, the nanoparticle trajectories in the stationary medium velocity field were determined. In both the simulation and the experiment, silver particles with a density \( \rho_s \) and a diameter \( d_p \) of 10.5 g/cm\(^3\) and 45 nm, respectively, were used. In the developed model, nanoparticles were released in a combination chamber at a velocity equal to the velocity of the carrier gas. Trajectories of the nanoparticles in the nozzle and during their deposition on the substrate were determined. To compute the particle trajectories from the velocity field obtained earlier, the following forces acting on the particle were taken into account:

Drag force [8]:

$$\vec{F}_{\text{Drag}} = \frac{1}{\tau_p} m_p (\vec{u} - \vec{v}); \quad \tau_p = \frac{\rho d_p^2}{18 \mu}$$

(3)

Saffman force [9]:

$$\vec{F}_{\text{Saff}} = -20.3d_p^2L_v \left( \mu p \frac{\vec{u} - \vec{v}}{|\vec{u} - \vec{v}|} \right)^{1/2}; \quad L_v = (\vec{u} - \vec{v}) \times \text{rot}(\vec{u} - \vec{v})$$

(4)

where \( m_p \) is the particle mass, \( \vec{v} \) is the particle velocity, \( d_p \) is the particle diameter.

Thus, as a result of the second stage of modeling, the positions of the nanoparticles on the substrate are determined. The line interval in which 68.2% of the particles lie (± σ from the average position) is a "contact spot" that determines the size of the structures formed. The dimensions of the contact spot were further compared to the width of the printed line, measured with an optical microscope in the real experiment.

3. Experimental

In order to verify the correctness of the model, we conducted a series of real experiments. We used the multi-spark discharge generator with a tube furnace to form silver nanoparticles [10]. The parameters of the m-SDG operation were set to generate nanoparticles with an average diameter of 45 nm. The carrier flow rate of argon \( Q_c \) was supplied to an internal axisymmetric channel. To the external conically converging axisymmetric channel, the sheath gas \( Q_s \) was supplied. Then the primary collimation of the flow took place in the combination chamber, and the final focusing of the nanoparticle beam occurred in the nozzle with an outlet diameter \( D_n = 100 \) μm. A focused beam of particles was deposited on the moving glass substrates. The speed of the substrates \( v_s \) was 65 μm/s. Thus, the parameters of the experiment on the focusing and deposition of nanoparticles replicated the parameters of the simulation. The width of the printed lines \( W_p \) was measured, using digital microscope VHX-1000.
4. Results and discussions

Figure 1 (b) shows the computed and the experimental dependence of the printed line width \( W_p \) on the sheath flow rate \( Q_{sb} \). Also presented are the computed trajectories of particle motion during the focusing and deposition process in the dry aerosol printing method (Figs 2a, b and c) and optical images of the lines formed from Ag nanoparticles deposited on the glass substrates (Figures 2d, e and f). Figures 1 (b) and 2 (a, b, d and e) show that, both in the model and in the experiment, with an increase in the sheath gas flow rate \( Q_{sb} \) from 90 to 150 sccm, the formed line width \( W_p \) decreases, indicating a qualitative agreement between the model and the experiment.

\[ Q_{sh} \, SCCC \]

Figure 1(a, b). (a) The drawing of a part of the printing head and the nozzle, used for the simulation; (b) The dependence of the printed line width on the sheath flow rate \( Q_{sb} \).

From Fig. 1 (b) and 2 (c and f) it is also seen that with the sheath gas flow rate \( Q_{sb} > 150 \) sccm, the results of the simulation and the real experiment differ qualitatively. This discrepancy, as well as the quantitative differences in the values of the line width of the simulation and the real experiments by several tens of percent, are probably due to the imperfections of the developed model, which does not take into account the three-dimensional nature of the nanoparticle focusing and deposition process. In particular, in the simulation, an increase in the printed line width \( W_p \) is observed with an increase in the sheath gas flow rate \( Q_{sb} > 150 \) sccm. At the same time, in the experiment, defocusing of the beam is not observed up to \( Q_{sh} = 190 \) sccm, and, consequently, the width of the formed \( W_p \) structures does not increase, but on the contrary decreases, with increasing the sheath flow rate \( Q_{sh} \), see Fig. 1 (b) and Fig. 2 (d, e, and f). Thus, a satisfactory qualitative agreement between the results of the simulation and the experiment is established for the nanoparticle focusing and deposition process at the sheath flow rate \( Q_{sh} \) of up to 150 sccm. At the same time, for sheath flow rate \( Q_{sh} > 150 \) sccm, the applicability of the developed model is limited.
Figure 2(a) – (f). (a, b, c) Computed particle trajectories in the deposition process; (d, e, f) The images of the printed lines taken with a digital microscope.

5. Conclusion
A computer model has been developed of the dry aerosol printing process, which allows to determine the size of the microstructures formed from nanoparticles from the printing process parameters, specifically the sheath gas flow rate. Development of the model was based on specifying the gas passage geometry and solving the system of equations to determine the trajectories of Ag nanoparticles up to 45 nm in diameter in the process of focusing and deposition on the surface of the substrate via a coaxial nozzle with an outlet diameter of about 100 μm. From the comparison of the results of the model and the experiment, it is found that a qualitative agreement between the model and the experiment is present with the sheath flow rate of up to 150 sccm.

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