Numerical Approach to Simulation of Nanoprinting Processes

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***Abstract* – This work-in-progress paper proposes a new numerical approach for the simulation of technological process of obtaining surfaces with given properties. This problem is relevant for many industrial applications. In medicine, nanotechnology enables us to create plasters, to implement bioprinting or to construct microsensors that will be used to detect cancer cells in the body. The paper describes a numerical method that helps to analyze different possibilities of producing functional surfaces coated with noble metal nanoparticles. Such surfaces may have many uses. Firstly, it is known that silver, aurum and other noble metals have a strong antibacterial effect. Secondly, the electrical conductivity of a noble metal is greater in comparison with the other metals. A set of numerical experiments have been done and their results are reported in this work.**

Keywords – multiscale mathematical models; numerical methods; nanotechnology problems; noble metal nanoparticles; nanoprinting in medical applications.

I. INTRODUCTION

In the late 2000s and early 2010s, in most developed countries, the potential for further growth of productivity in the world economic and technological sectors was limited [1]. Recovery of high rates of productivity in the economy and its profit can not be achieved only through macroeconomic measures. At present, the answer to the challenge of preserving competitiveness and achieving high rates of productivity should be given by the scientific, technological and innovation policies pursued by industrialized countries. The purpose of these policies is to stimulate development and implementation of advanced technologies, whose performance significantly exceeds the characteristics of traditional technologies.

The traditional and new mathematics, mathematical methods, numerical methods based on multiscale models, differential equations and classical physics underlie the development of the novel technologies.

Nowadays, clearly identified directions that can be considered technologically mainstream include: information technology, biotechnology, nanotechnology, ecological technology, and cognitive technology. They represent a new technological interface between humans and their environment [2]. The progress of these directions defines technological development and its rate corresponding to the modern world challenges.

Nanotechnology plays an important role in industrial and natural processes in a variety of fields including engineering, production of consumer goods, public health and biology. The creation of micro- or nanostructures on the substrate surface not only changes its topography, but can substantially modify the properties of the substance. By creating structures similar to natural objects, we can control their properties without changing their chemical nature.

Multicolored butterfly wings are painted in all colors of the rainbow without any paints, geckos know how to run on steep walls without using glue, the leaves of some plants can purify themselves and repel droplets of water without chemical treatment. All this is possible thanks to the hierarchically structured topography of biological objects and can be reproduced with the help of nanotechnology [3]-[7].

The typical size of noble metal particles is equal to 5-50 nm. These nanoparticles are the strongest biocidal agents and are used in biosensors and numerous assays. Nanostructure materials with noble metal nanoparticles can be used as biological markers for quantitative detection. For example, silver nanoparticles are incorporated in apparel, footwear, paints, wound dressings, appliances, cosmetics, and plastics for their antibacterial properties [8]. The unique properties of silver nanoparticles make them attractive for numerous areas.

It is known that materials can be modified with noble metal nanoparticles, using plasma treatment or cold gas spraying. In contrast to other technologies, this enables the creation of materials with different bactericidal properties and also high hydrophilicity/hydrophobicity. For example, the ability to absorb body moisture is an important hygienic indicator.

In this paper, we study the nanoprinting processes at low and room temperatures (100-350 K). Cold rarefied gas accelerated to supersonic speed is used for transportation of noble metal nanoparticles to a hot substrate.

In our previous works, we analyzed jet flows, streams in microchannels and other gas dynamic problems using a new multiscale approach [9]-[12]. This approach combines the traditional hydrodynamic models (we use quasigasdynamic equations [13],[14]) with Newton's dynamics equations for individual particles. In this paper, we use direct molecular dynamic simulation [15]-[18].

This paper is organized as follows: Section II states the current problem and gives some literature references to preview works. In Section III, we describe what methods are used in the research, and we consider the main

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macroparameters of the system. Section IV presents the preliminary results of the current research. Section V presents conclusions that can be drawn from the testing results and addresses future work as well. The future study will exceed the scope of this research. Also, the next steps and future plans of this study are described in this section.

In the paper an approach for the cold gas spraying process of the nanoparticles on substrate is discussed.

II. STATEMENT OF THE PROBLEM

In the present work, the process of acceleration of a metallic nanocluster by a supersonic gas flow is considered. The purpose of this particular procedure is to allow the metal clusters to reach a predetermined constant velocity, which will allow these clusters to adhere to a hot substrate in case of contact with it. The procedure is illustrated in Figure 1, which shows a fragment of the spraying system.

To describe the acceleration of the nanocluster, we used the equations of two-component molecular dynamics [18]:

$$m_l \frac{d\mathbf{v}_{l,i}}{dt} = \mathbf{F}_{l,i}, \quad \frac{d\mathbf{r}_{l,i}}{dt} = \mathbf{v}_{l,i}, \quad i = 1,...,N_l, \quad l = a,b, \quad (1)$$

where i is the particle number, l is the particle type (a – molecules of gas, b – atoms of metal in the nanocluster), N_l is the total number of particles of type l, m_l is the mass of particle of type l, $\mathbf{r}_{l,i} = \left(r_{x,l,i}, r_{y,l,i}, r_{z,l,i}\right)$ and $\mathbf{v}_{l,i} = \left(v_{x,l,i}, v_{y,l,i}, v_{z,l,i}\right)$ are the position vector and the velocity vector of the i-th particle of type l, $\mathbf{F}_{l,i} = \left(F_{x,l,i}, F_{y,l,i}, F_{z,l,i}\right)$ is the resultant force acting on this particle.

The forces include the component of i-th particle interaction with the surrounding particles and the component responsible for external action:

$$\mathbf{F}_{l,i} = -\nabla_{\mathbf{r}_{l,i}} U + \mathbf{F}^{ext}_{l,i}, \quad i = 1,...,N_l, \quad l = a,b. \quad (2)$$

Here, $\mathbf{F}^{ext}_{l,i}$ is the force of interaction with the environment, U is the total potential energy and it depends on choosing the interaction potential of molecules. The potential energy of the system is represented as a function that depends on the coordinates of considered particles and describes the interaction between the particles of the system. Selecting a specific type of interaction potential is based on a comparison of the mechanical properties of the computer model of potential and real material. To solve equations (1) and (2), it is necessary to consider all options of interaction l with l' for $l = a,b$ and $l' = a,b$. As an example, the potential functions for modeling the interactions between the gas molecules and the metal atoms of the nanocluster can be considered, which were used in [19].

For closure of (1) and (2), the periodic boundary conditions were used.

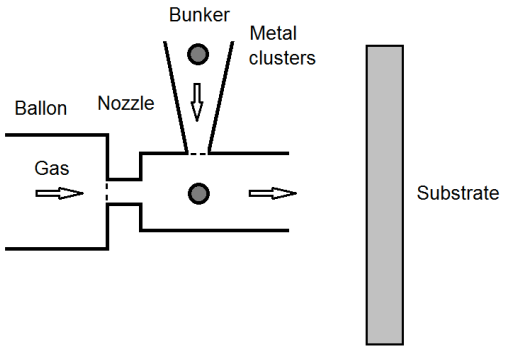

Figure 1. Fragment of spraying microsystem.

An initial state of the gas and the metal systems corresponded to the condition of thermodynamic equilibrium at a predetermined temperature and pressure.

III. METHOD OF STUDY

A numerical algorithm for integration of equations (1) and (2) is based on well known Verlet's scheme [20]:

$$\begin{cases} \mathbf{v}^{n+1/2}_{l,i} = \mathbf{v}^{n}_{l,i} + \dfrac{\mathbf{F}^{n}_{l,i}}{2m_{l,i}}\Delta t, \quad \mathbf{r}^{n+1}_{l,i} = \mathbf{r}^{n}_{l,i} + \mathbf{v}^{n+1/2}_{l,i}\Delta t, \\ \mathbf{v}^{n+1}_{l,i} = \mathbf{v}^{n+1/2}_{l,i} + \dfrac{\mathbf{F}^{n+1}_{l,i}}{2m_{l,i}}\Delta t, \quad i = 1,...,N_l, \quad l = a,b. \end{cases} \quad (3)$$

Here, Δt is the integration step (in time), n is the step number, $\mathbf{F}^{n+1}$ is the value of the force at this step.

At the initial time, the coordinates and velocities of all particles are set. Further, at each time step, the equations of motion are solved; new values of the force vectors, new coordinates and velocities are computed. Calculations are carried out taking into account the boundary conditions and the external impact on the system in areas where this impact is present.

Kinetic energy of thermal motion E_T, kinetic energy E_K and total energy E of the system are calculated separately for particles of each type $l = a,b$ as follows:

$$E_K = \sum_i E_{K,l,i}, \quad E_T = \sum_i E_{T,l,i}, \quad E = E_K + U,$$
$$E_{K,l,i} = m_{l,i}\left|\mathbf{v}_{l,i}\right|^2/2, \quad E_{T,l,i} = m_{l,i}\left|\mathbf{v}_{l,i} - \mathbf{v}_l\right|^2/2, \quad (4)$$
$$\mathbf{v}_l = \frac{1}{N_l}\sum_i \mathbf{v}_{l,i}, \quad i = 1,...,N_l, \quad l = a,b.$$

Here, $E_{K,l,i}$ is the kinetic energy of the particle with number i, $E_{T,l,i}$ is the thermal kinetic energy of the particle with number i, $\left|\mathbf{v}_{l,i}\right|$ is the velocity vector length of i-th particle

of l type, $\mathbf{v}_l = \left(v_{x,l}, v_{y,l}, v_{z,l}\right)$ is the center-of-momentum frame velocity for particles of type $l = a,b$.

Gas or metal particle system temperature T and pressure p are defined as follows:

$$T = \frac{2}{d}\frac{\langle E_T \rangle}{N k_b}, \quad p = \frac{1}{3}\left(p_{xx} + p_{yy} + p_{zz}\right), \\ p_{\alpha\alpha} = \frac{1}{V}\sum_i m_i \left(v_{i,\alpha} - v_\alpha\right)^2 + \frac{1}{V}\sum_i \sum_{j>i} r_{ij,\alpha} \cdot F_{ij,\alpha}. \quad (5)$$

Here, d is the number of particle freedom degrees, k_b is the Boltzmann constant (further unless otherwise is stated $d = 3$), V is the volume of the system, $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, $\mathbf{F}_{ij}$ is the force of interaction between i-th and j-th particles, α is coordinate x, y or z accordingly. The particle type index has been removed from the formula for clarity of expression.

The initial state of the gas and metal microsystem was realized by thermostating.

IV. Results and Disscussion

As a model problem, the problem of acceleration of a nickel cluster by nitrogen molecules was considered. The dimensions of the cubic-shaped cluster were 24^3 crystals or 8.475^3 nm^3, and the number of atoms was 55296 (see Figure 2). The initial position of the cluster center was at the point $\left(266.97, 34.14, 34.14\right)$; sizes were measured in nanometers. The acceleration was carried out by injecting a small portion of gas into the system. In this case, a gas microsystem containing 82904 molecules was used. The microsystem was under normal conditions ($T = 273.15\,K$, $p = 101325\,Pa$). Approximately a half of these molecules were pre-accelerated to speeds of 14 Mach (see Figure 3).

The performed calculation was related to the analysis of the evolution of a shock wave and its interaction with the nanocluster and resting gas molecules. Figure 3 shows the longitudinal velocity distributions of the gas near the region occupied by the nanoclusters; values are averaged over the coordinate y. They illustrate some details of the acceleration process. At the beginning of this process, the front of the shock wave is scattered near the cluster. But the cluster itself does not move much. Then, it begins to accelerate slowly and evenly up to a certain limiting speed (see Figures 4 and 5). The magnitude of this velocity is related to the amount of gas incident on the cluster and its total momentum. If the value of the total momentum of the gas is small, it will take a very long time to accelerate the system to a certain average speed. From the law of conservation of momentum, we can estimate the value of the total average velocity:

$$\mathbf{v}^{(\infty)} = \frac{m_a N_a^*}{\left(m_a N_a + m_b N_b\right)}\mathbf{v}^{(0)}, \quad (6)$$

where $\mathbf{v}^{(0)}$ is the average initial velocity of accelerated nitrogen molecules, N_a^* is the number of such molecules.

The numerical algorithm was implemented as a parallel program using the MPI [21] and OpenMP [22] standards. Model calculations were performed on K60 cluster with processors Intel Xeon E5-2690 v4 @ 2.60GHz and a total performance of 60 TFlops.

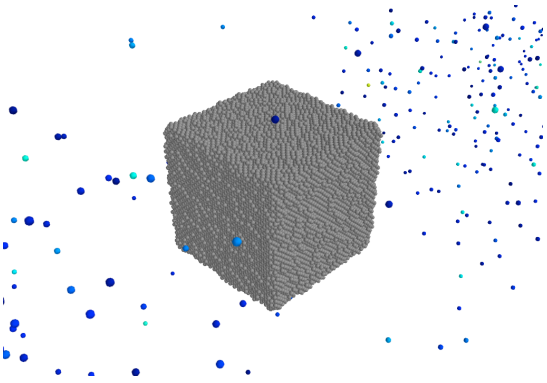

Figure 2. 3D image of the nanocluster and gas molecules at the beginning of the acceleration process.

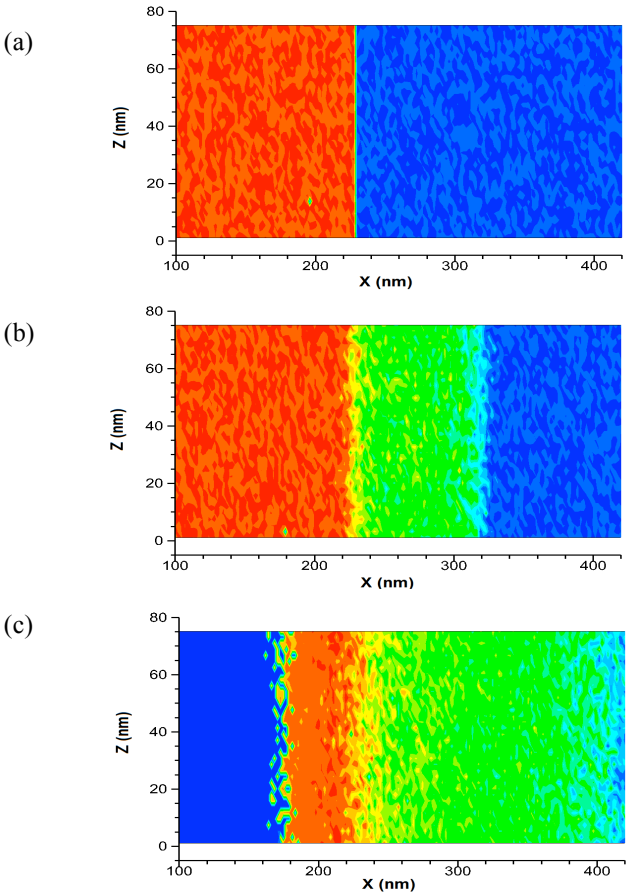

Figure 3. Distributions of the longitudinal velocity of the gas averaged over the coordinate y at time points 0, 18, 38 ps (a, b, c).

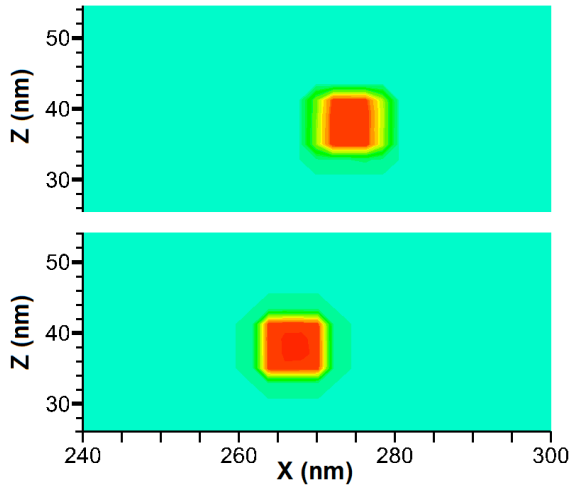

Figure 4. Position of the nanocluster at initial time (from below) and at time point 350 ps (from above). Coordinates are measured in nanometers.

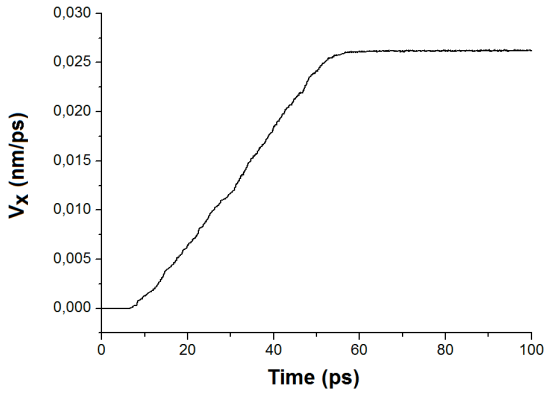

Figure 5. Evolution of the longitudinal velocity of the cluster.

V. Conclusion and Future Work

In this paper, we considered only the first stage of the process of spraying and deposition of nanoparticles on a substrate associated with the acceleration of a single nanocluster. The numerical approach based on the direct molecular modelling was used for this purpose. The continuation of this work will be connected both with the interaction of the cluster accelerated to a certain velocity with the substrate, and the general spraying processes, in which a lot of clusters participate. In the future, we will consider the nanoparticles of other metals. In this general problem, it is proposed to use the multiscale technology developed in previous works of the authors.

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