

# Mathematical Model of Motion of Modifying Powder Particles in the Shielding (Carrier) Gas

M A Kuznetsov <sup>a</sup>, A V Kryukov <sup>b</sup>, A G Krampit <sup>c</sup>, E A Zernin <sup>d</sup>, I D Sadykov

Yurga Institute of Technology (Affiliate) of Federal State Autonomous Educational Institution of Higher Professional Education “National Research Tomsk Polytechnic University”, Yurga, Russia (652050, Yurga, 26, Leningradskaya str.)

e-mail: <sup>a</sup>kyznechik\_85@mail.ru, <sup>b</sup>earendill@mail.ru, <sup>c</sup>akrampit@mail.ru, <sup>d</sup>yuti\_sp@bk.ru

**Abstract:** The paper gives some consideration to the model of including ultradisperse modifiers into the surface layer of material through the shielding (carrier) gas. It has been revealed this technique of inclusion necessitates ultradisperse particles to be 100 – 150 nm for their efficient transfer by the shielding (carrier) gas. Particles of smaller dimensions can't get in a jet of the shielding (carrier) gas. Probability of such defect as “impurity” occurs provided that particles are over 150 nm.

## 1. Introduction

Low stability of equipment against intercrystalline corrosion, especially in zones affected by high temperature in the process of manufacturing is a vital problem of pharmaceutical, chemical, power, nuclear and food industries. Therefore, in recent years researchers have been focusing their attention on the issues of increase in corrosion resistance by means of modifying layers. Obtaining special properties of the surface via modifying is inseparably linked with solution of the problems how to produce, test modifying powders and choose the method of their inclusion into the layer to be processed.

Authors of the paper deal with the technique of ultradisperse powder inclusion through the shielding (carrier) gas; this technique makes it possible to control concentration of ultradisperse particles in the shielding (carrier) gas [1]. The authors decided to specify the dimensions of modifier particles by means of mathematical simulation.

Mathematical simulation has been developed successfully and now it is considered a powerful tool to study non-linear problems in various fields of science. If natural experiment is impossible, complicated or cost intensive mathematical simulation is used [2,3,4,5,6,7,8].

Development of computer engineering provides excellent perspectives for application of complex models displaying multiple-factor character and interconnection of different physical processes and phenomena [9].

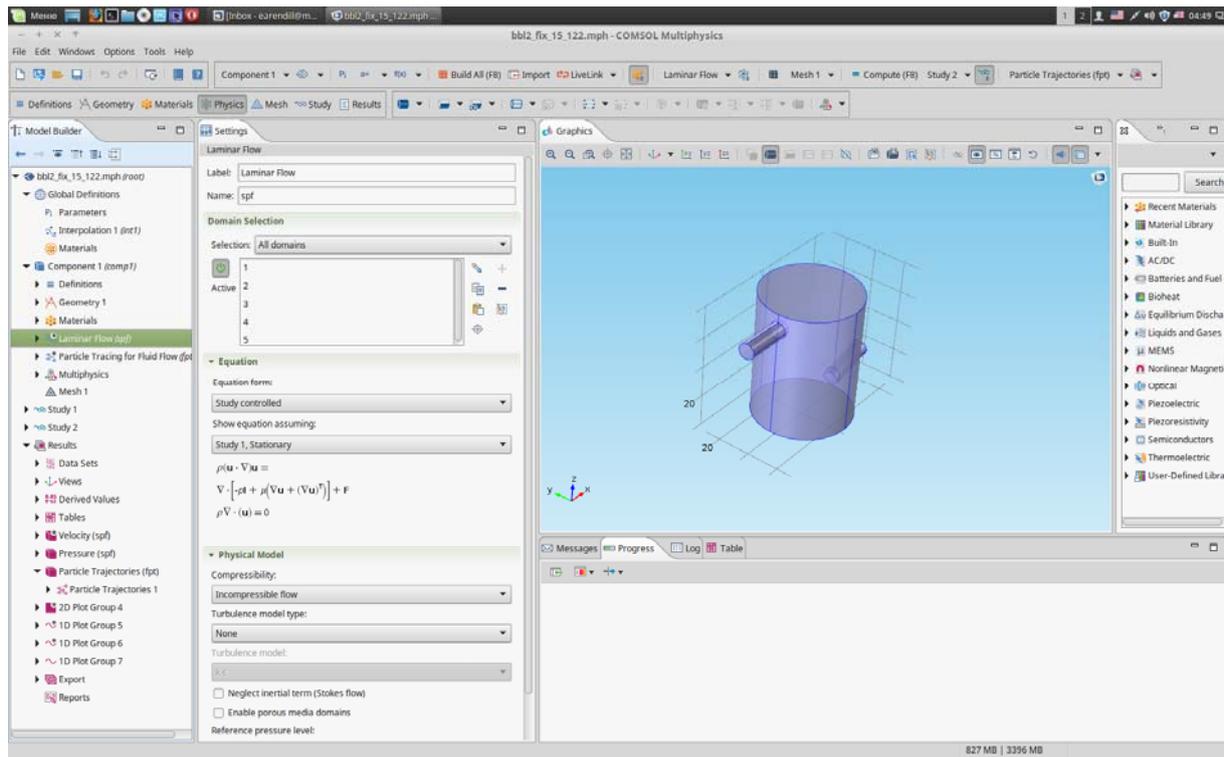
Software package CONSOL “Multiphysics” intended for simulation of various physical processes, systems and their interconnection is a powerful simulation tool. “Consol” is a flexible platform allowing adapting model to real conditions, supplementing or modifying some physical processes described both by standard and set up by the user interfaces based on the system of differential



equations in partial derivatives. As the consequence, a model maximally resembling the reality can be obtained.

## 2. Mathematical statement of the problem

Software package “CONSOL Multiphysics” was used to develop a computer model in the course of work. We calculated particle distribution in the volume and their mechanical trajectory on the base of gas jet rate distribution and data on particles inside the mixer (Fig. 1).



**Figure 1** Window of software “CONSOL Multiphysics” to calculate the trajectory

The aim defined in the paper was attained in two steps:

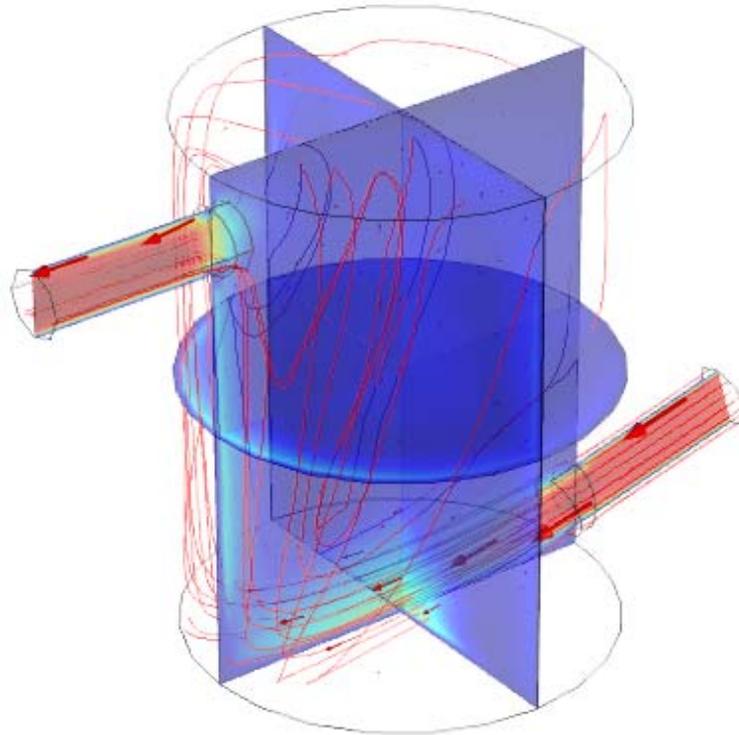
1. Simulating argon supply into the mixers;
2. Simulating the trajectory of particles in the gas jet.

1. Argon supply into the mixers was simulated on the base of differential equation of laminar flow (1).

$$\rho(u \cdot \nabla)u = \nabla \cdot [-\rho i + \mu(\nabla u + (\nabla u)^T)] + F \quad (1)$$

where  $\rho \nabla \cdot (u) = 0$ ,  $\rho$  – gas density;  $u$  – gas rate component;  $\nabla$  – inverted delta,  $\mu$  – dynamic viscosity;  $T$  – ambient temperature.

The following boundary conditions were determined for modelling: inlet conditions include  $u = -U_0 n$ , where  $U_0$  specifying according to consumed shielding gas. Outlet conditions correspond to zero pressure. The rate distribution of shielding (carrier) gas jet is depicted in Figure 2.



**Figure 2** Distribution of gas jet rate

2. Simulating the trajectory of particles in the gas jet.

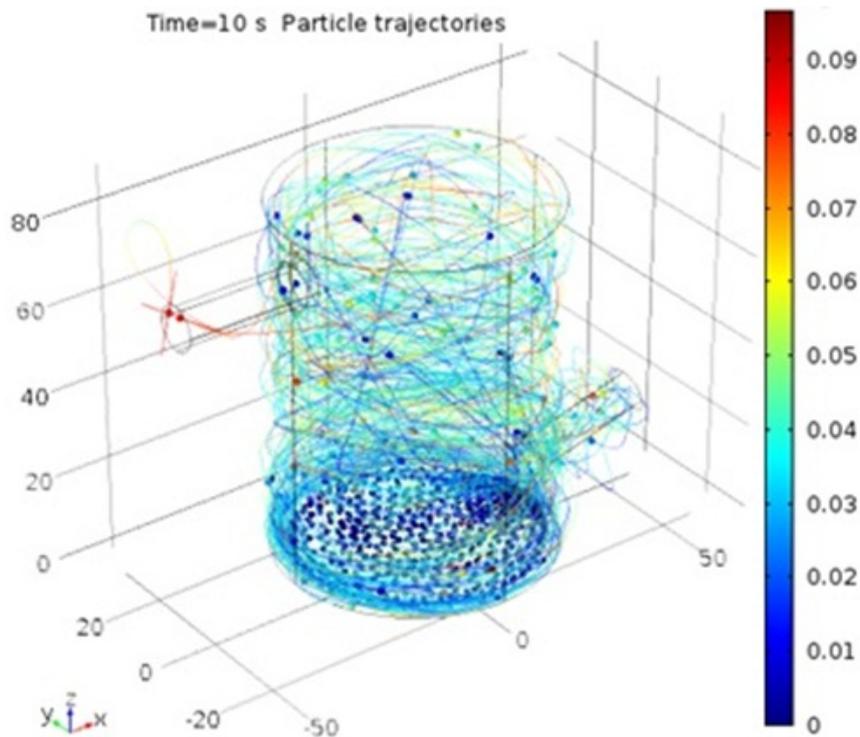
The motion of particles in the jet of shielding (carrier) gas can be described by equation (2)

$$\frac{d(m_p v)}{dt} = F_i \quad (2)$$

The following boundary conditions were specified for modelling: initialization of particles at the zero second in terms of finite element mesh; driving force  $F = \frac{1}{\tau_p} m_p (u - v)$ ;  $\tau_p = \frac{\rho_p d_p^2}{18\mu}$

where  $m_p$  – particle mass;  $u$  – particle rate component;  $v$  – jet rate component,  $\rho_p$  – density of a particle;  $d_p$  – diameter of a particle.

The motion of particles in shielding (carrier) gas is presented in Figure 3.



**Figure 3** Motion of particles in the jet of shielding (carrier) gas

### 3. Results and Discussion

The obtained model was applied to study 4 sizes of moving particles (below 100 nm, 100-150 nm, 200-500 nm, and over 500) of modifying powders (tungsten, molybdenum, aluminium oxy-hydroxide).

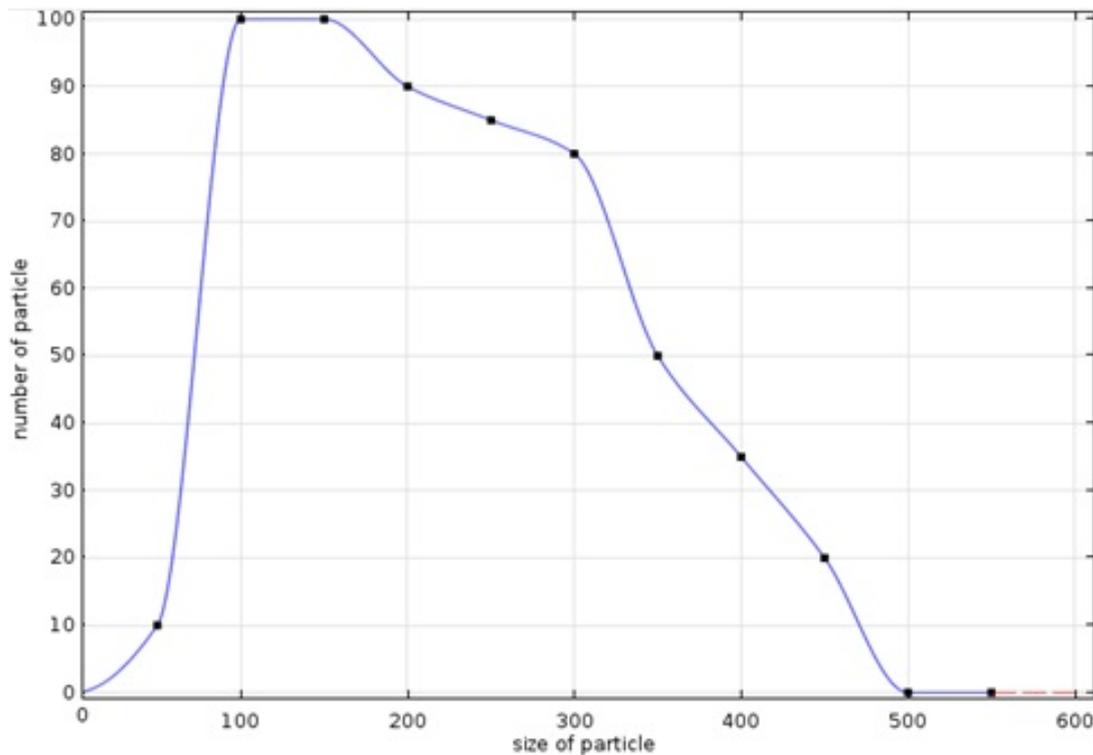
In view of calculations the total amount of inlet initialized particles was estimated, as well as the percentage of particles transferred by jet to the outlet. Figure 4 presents the dependence of particles transferred by jet on their size. As the result of obtained data analysis, 100 to 150 nm particles are required for their efficient transfer.

The outcomes of mathematical simulation point to the following fact: maximum 5 of 1000 initialized in the mesh particles get into the jet of shielding (carrier) gas for 10 seconds provided that their size does not exceed 100 nm. If the particles are 100 to 150 nm, 100 of them get into the jet of shielding gas, if the sizes are 200 to 500 nm, their number in the shielding gas goes up to 50, and such defect as “impurity” is probable, particles 500 nm and above are not transferred into the jet of shielding (carrier) gas because of their mass.

Then, we studied the range of particle dimensions 100 to 150 nm to determine the efficient size of particles of the following modifying powders: tungsten, molybdenum, aluminium oxy-hydroxide). Table 1 provides main results of based on the above ideas calculations of particle motion of modifying powders in the jet of shielding (carrier) gas in the mixer according to the dimensions of particles.

Table 1 – Efficient technological parameters of modifying powder particles

Modifying powder	Size, nm	Mean density, g/cm <sup>3</sup>	Consumption, mg/m
Tungsten	122	15	4
Molybdenum	127	4	4
Aluminium oxy-hydroxide	150	0.4	4



**Figure 4** The number of particles in shielding (carrier) gas determined by the size of a particle

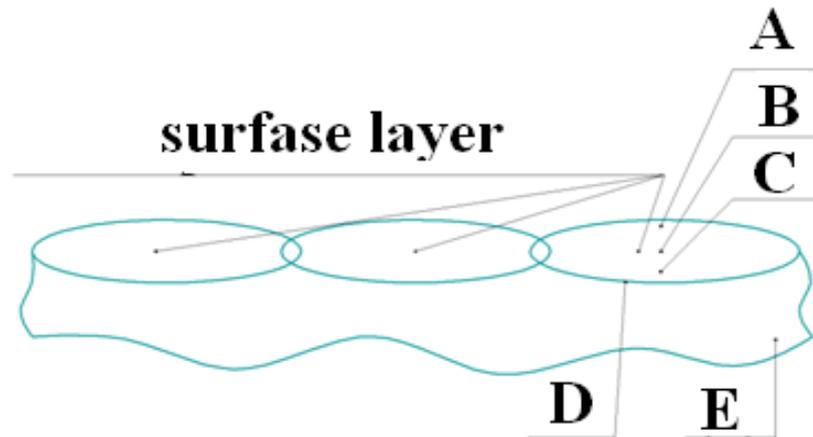
Production of powders by electric explosion of conductors relied on the carried out simulation. This method allows varying dispersibility of the powder by changing both physical (diameter, length of the wire to be exploded, gas pressure in the facility) and electro-physical parameters (operating voltage, capacity, circuit inductance), as the consequence, energy applied to the conductor under electric explosion [10].

For the purpose of work we used tungsten (W) and molybdenum (Mo) powders produced by electric explosion of conductor and aluminium oxy-hydroxide  $\text{AlO}(\text{OH})$  produced by electric explosion of conductor and subjected to thermal hydrolysis.

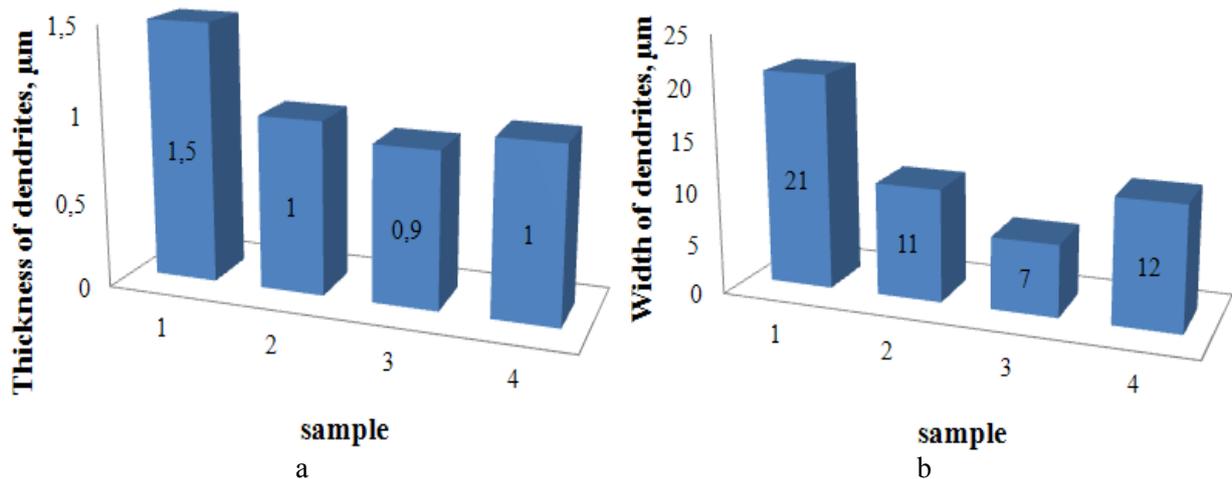
Experiments pointed at the possibility of significant influence on grain dimensions and corrosion resistance of the arc-processed surface via changing powder concentration in the carrier gas [11,12,13].

The surface layer, as we have identified, has a laminated structure: a sub-layer of fine polyhedral austenite grains with the spots of non-oriented dendrites adjacent to the free surface, a sub-layer of short and thick non-oriented dendrites, and a sub-layer of extended oriented dendrites. The thickness of sub-layers depends on powder modifier (Figure 5).

We have found out modifying the surface layer by ultra-disperse powders  $\text{AlO}(\text{OH})$ , W and Mo at the rate of 4 mg per meter of the layer has the most pronounced effect of modifying the surface layer in the system Fe-C-Cr-Ni-Ti due to arising in the melt additional centres of crystallization – inoculators in crystallizing metal. Mean thickness of dendrite gets reduced by the factor of 1.5 - 2 (30-40%), its width is decreased by the factor of 2 - 3 (45-55%) (Figure 6).



**Figure 5** – A layout chart of zones in the microstructure of the surface layer to be examined: A – a sub-layer of fine polyhedral austenite grains with the spots of non-oriented dendrites, B – a sub-layer of short and thick non-oriented dendrites, C – a sub-layer of extended dendrites, D – a surface – base layer transition zone, E – base metal

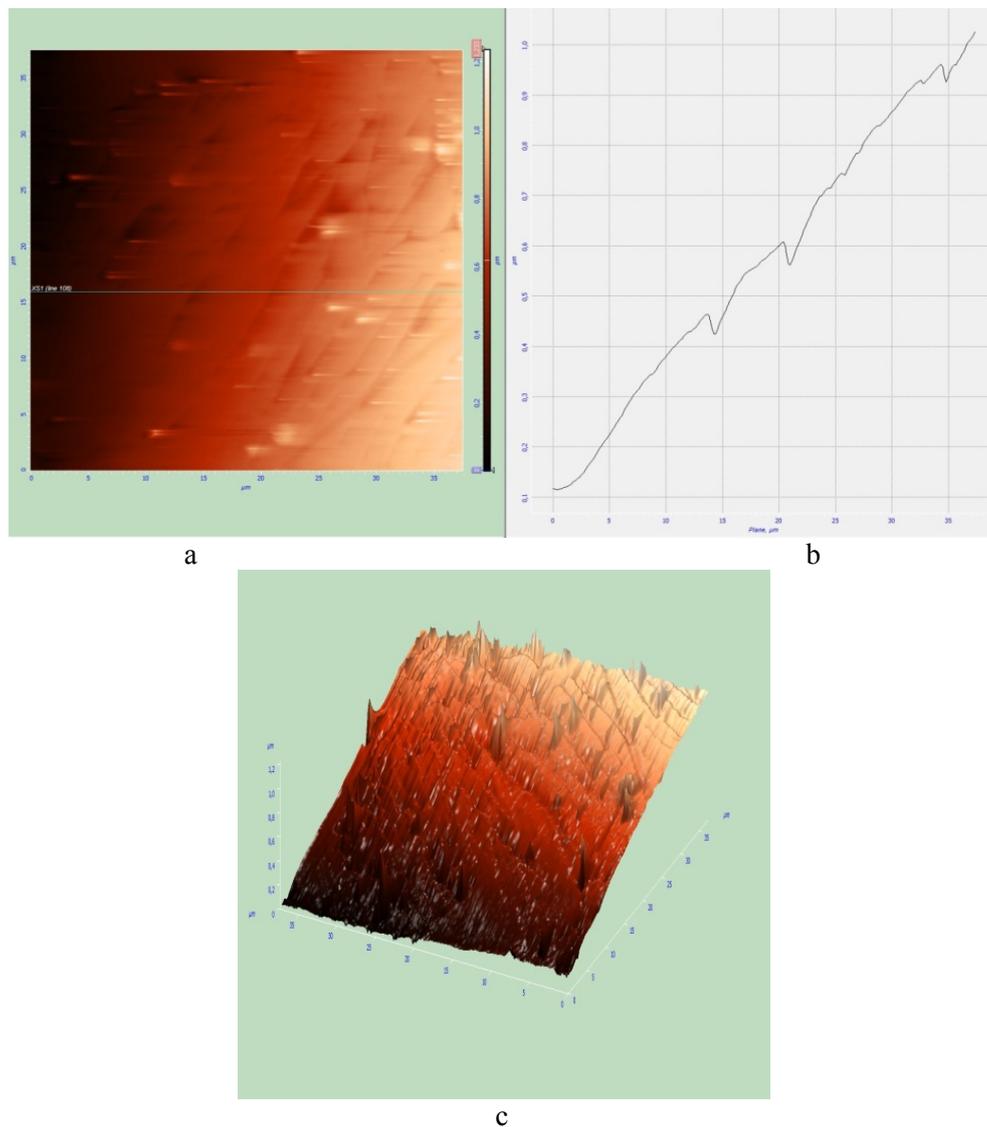


**Figure 6** Dendrite dimensions: a – thickness of dendrites, b – width of dendrites  
 1 – without powder; 2 – with powder W; 3 – with powder AlO(OH);  
 4 – with powder Mo

Polyhedral grain boundaries are clear and their width did not increase after corrosion resistance tests. The structure of the surface layer modified by ultradisperse powders did not change somehow both near the melting border and in the bulk.

Therefore, high resistance to intercrystalline corrosion of the surface layer modified by ultradisperse powders was determined when applying standard metallographic methods. Atomic force microscopy tests of the surface layer structure confirm the results of metallography: the surface layer does not tend towards intercrystalline corrosion.

Grain boundaries do not really change. Etching was carried out not on grain boundaries but on their whole surface. The surface of grains was etched less or more according to their orientation. As the consequence, grooves formed between the grains (Figure 7).



**Figure 7:** a – AFM 2D image of welded metal,  
 b – profilogram on the line marked in the image:  
 c – AFM 3D image of the same zone

The sample modified by ultradisperse tungsten powder had the lowest jog; that is why; it was less etched under corrosion tests.

### Conclusions

1. The mathematical model of motion of modifying powder particles in a streamline flow of a carrier gas has been proposed.

2. Efficient dimensions of particles for transferring a modifier by gas jet were specified on the base of proposed model. The minimum size of particles is 120 nm as smaller particles are not transferred into the jet of a carrier gas. If the size of particles exceeds 150 nm such defect as “impurity” is probable. Therefore, particles are to be 120 to 150 nm.

3. Rational technological parameters (dimensions of particles, their mean bulk density) of three type modifiers for austenite steels were determined according to the number of particles transferred by the gas jet: tungsten (W) – 122 nm, 15 g/cm<sup>3</sup>; molybdenum (Mo) – 127 nm, 4 g/cm<sup>3</sup>; aluminium oxy-

hydroxide (AlO(OH)) – 150 nm, 0.4 g/cm<sup>3</sup>. That is, the number of particles transferred by the gas jet is to tend towards a maximum.

4. Modifying the surface layer by ultra-disperse powders AlO(OH), W and Mo at the rate of 4 mg per meter of the layer has the most pronounced effect of modifying the surface layer in the system Fe-Cr-Ni-Ti due to arising in the melt additional centres of crystallization – inoculators in crystallizing metal. Mean thickness of dendrite gets reduced by the factor of 1.5 - 2 (30-40%), its width is decreased by the factor of 2 - 3 (45-55%).

5. It has been revealed, key factors for determining the resistance to intercrystalline corrosion of permanent joints are composition and structure of the heat-affected zone, its stability under operational influence as well. Samples produced by inclusion of nano-structured powders into the welded metal are the most corrosion resistant in view of structure and metal stability in the heat-affected zone.

## References

- [1] Kuznetsov M.A., Barannikova S.A., Zernin E.A., Filonov A.V., Kartsev D.S. 2015 Applied Mechanics and Materials Methods for defining the concentration of nanostructured powders in protective gas and its effect on the microstructure of deposit metal 770 pp. 28-33.
- [2] Mazhukin V.I., Shapranov A.V., Perezhigin V.E. 2012 Mathematical simulation of thermophysical properties, heating and melting processes of metals by the method of molecular dynamics // X International Seminar "Mathematical Models & Modelling in Laser-Plasma Processes & Advanced Science Technologies, Vol XXIV pp. 47-65.
- [3] Mazhukin V.I., Shapranov A.V. 2012 Mathematical simulation of metal heating and melting. Part I. Model and Computational algorithm // Preprints of Keldysh Institute of Applied Mathematics 31 – 27 p.
- [4] Chinakhov D.A., Vorobjev A.V., Tomchik A.A. 2013 Materials Science Forum Simulation of Active Shielding Gas Impact on Heat Distribution in the Weld Zone 762 pp 717-721.
- [5] Chinakhov D.A., Vorobjev A.V., Gotovshchik Y.M. 2014 Applied Mechanics and Materials Simulation of wind Influence on the thermal processes in gas-shielded welding 682 pp. 91-95.
- [6] Krampit M.A., Krampit N.Y. 2015 Applied Mechanics and Materials Electronic circuit design of power supplies for welding in Ispice Iv program // 770 pp. 323-327.
- [7] Temlyantsev M.V., Starikov V.S., Kondratiev V.G. 2000 Proceedings of the higher educational institutions. Iron and steel modeling of temperature fields and resistance to deformation in cylindrical workpieces by heating with a hot tenements for rolling 6. pp. 51-54.
- [8] Temlyantsev M.V., Starikov V.S. 2000 Proceedings of the higher educational institutions. Iron and steel calculation of temperature fields in prismatic workpieces during thermal cycling with 2. pp. 42-45.
- [9] Makhnenko V.I. 2002 Perspectives of mathematical simulation and information technologies in welding and related processes // Mathematical simulation and information technologies in welding and related processes: Proceedings of International Conference; Paton Welding Institute Kiev pp. 3-11.
- [10] Yavorovsky N.A. 1996 Proceedings of Higher Educational Institutions. Physics. Production of ultradisperse powders by electric explosion 4 pp. 114 – 136.
- [11] Kuznetsov M.A., Zhuravkov S.P, Zernin E.A., Kolmogorov D.E., Yavorovsky N.A. 2014 Advanced Materials Research Influence of Nanostructured Powder Modifiers on the Structure of a Welding Bead 872 pp. 118-122.
- [12] Kuznetsov M.A., Zernin E.A., Zhuravkov S.P., Yavorovsky N.A. 2014 Advanced Materials Research Influence of nanopowders on corrosion resistance of weltded joints 1040 pp. 837-844.
- [13] Kuznetsov M.A., Zernin E.A., Danilov V.I., Kolmogorov D.E., Zoubenko L.N. 2015 IOP Conference Series: Materials Science and Engineering Corrosion and mechanical properties of austenic steel weld joints 91 pp. 012010 doi:10.1088/1757-899X/91/1/012010.