Study of the Functional Characteristics of TiNi Coatings by the Computer-Aided Simulation Using Parallel Computing

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Abstract. The architecture and functionality of a program system that implements the paradigm of parallel execution of SIMD-tasks, in which a certain class of coatings with different parameter sets of particles sprayed onto the surface of technical products are simulated, is considered. Each SIMD-task uses a copy of the same computing module, which implements the computational foundations of a previously created software package for simulation the layered structure of a gas-thermal coating and calculating its functional characteristics. The program system allows you to run a series of computational experiments with the least amount of time due to the parallel running of SIMD-tasks for simulation a class of functional coatings, taking into account various spraying modes, and save electronic reports with illustrative research material in archival storage. The paper presents the results of simulation a class of coatings made of titanium nickelide (TiNi), taking into account various sets of "key physical parameters" (KPPs) of particles, characterizing different modes of coating spraying. In addition, based on the simulation results, an analysis was carried out of the variability of the coatings functional characteristics (porosity and adhesive strength of coatings, surface roughness of coatings) when varying the KPP-values in certain ranges. As a result of analyzing the simulation results of TiNi coatings and calculating their functional characteristics, optimal modes for the stable spraying of TiNi coatings on two types of substrates (on a Steel45 substrate and on a titanium substrate) were established.

Keywords: Program System, Computational Experiments, Parallel Computing, SIMD-Task, Simulation, Spraying, Gas-Thermal Coatings, Titanium Nickelide.

1 Introduction

In the field of materials science, methods and technologies for gas-thermal spraying (GTS) of functional coatings (on technical products), which are characterized by a high degree of wear resistance, resistance to shock mechanical and thermal influences, etc., have now been quite effectively developed. Effective GTS-technologies are the follow-

ing [1-3]: APS (atmospheric plasma spraying); D-gun spraying (detonation-gas spraying); HVOF-spraying (high velocity oxygen fuel spraying) and many other technologies that allow the formation of coatings from powders of metal, ceramic, or metal-ceramic particles (cermets).

Scientific publications and various monographs on this topic contain a fairly large volume of experimental data on the functional characteristics (physical properties) of gas-thermal coatings. However, so far such data have not been sufficiently systematized and, on their basis, a holistic understanding of the relationship between modes of spraying and the functional characteristics of the resulting coatings has not been formed. To solve this problem, the authors developed a program complex for simulation and designing the layered structure of gas-thermal coatings and calculating their functional characteristics [4, 5]. This program complex allows you to carry out sequentially one after another the computational experiments (CEs), corresponding to various sets of spraying modes parameters and initial data characterizing the physical properties of sprayed materials. However, the computational costs of performing computational experiments on modern computers are quite high (the time spent on one CE can reach several days). Therefore, the actual problem of increasing the computational efficiency of the software package was an attempt by the authors to develop a program system for parallel running of identical copies of a computing module that implements the computational foundations of the previously created software package for simulation the layered structure of gas-thermal coatings and calculating their functional characteristics. A series of CEs with a different sets of parameters corresponding to the spraying of a certain class of coatings is performed by the program system in parallel mode.

Turning to the history of the development of computer technology, in the first stages of its development with the use of computers in large scientific institutions, it became possible to develop programs that completely carry out the numerical solution of any particular version of a computational problem based on one set of data. When changing the data set, it was necessary to contact the computer center again with a request to complete the task. The results obtained were processed manually, then compiled into a report, and the missing intermediate values were supplemented by interpolation methods based on the calculated data.

Currently, the processor architecture in personal computers (PCs) is multi-core; processors and computers are combined into multiprocessor configurations in the form of large computing clusters and MPP systems. It became possible not only to increase the complexity of the problems being solved, but also to perform cycles of a large number of computational experiments (up to 1000 or more) using identical copies of one program with different sets of data (variable parameters – input data of a “typical” task). In addition, it is possible to summarize the calculation results into ready-made “electronic” reports. A cycle (series) of computational experiments (CEs), executed using a single program (for example, in Fortran, C/C++, etc.) with different sets of input data of the same structure and sizes, defines the so-called “class of similar SIMD-tasks".

This work aims to further improve and use for research in the field of materials science a program system, developed on the basis of the program complex previously created by the authors for simulation (computer-aided design) of gas-thermal coatings and calculating their functional characteristics (see Fig. 1). The program system makes

it possible to automate the running of a series of CEs with the processing of their results and the preparation of electronic reports with the least amount of time due to the parallel execution (running) of the corresponding class of similar SIMD-tasks. Computational modules (CMs) in SIMD-tasks are represented by the same program code, which is the computational basis of the program complex for coating simulation (Fig. 1), i.e. all CMs are identical software copies.

2 Brief Description of the Program Complex for Coating Simulation

The composition of the program complex [6] designed for coating simulation is shown in Fig. 1.

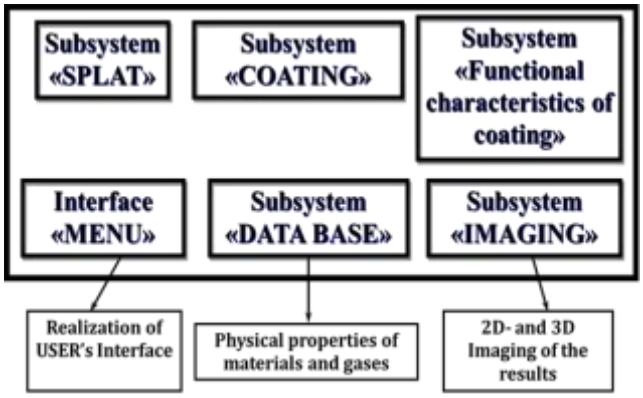

Fig. 1. Structure of the program complex for coating simulation and calculating their functional characteristics [6].

Let us consider the capabilities of the "SPLAT" subsystem and the "COATING" subsystem [4-6].

Subsystem "SPLAT" allows you to calculate the splat geometric characteristics (using the subsystem "DATA BASE"). The splats formed as a result of the collision of particles in the form of microdroplets of the melt with the base (substrate or pre-sprayed layer) with their subsequent spreading and solidification on the base (substrate). The calculation of the splat characteristics is carried out using a selected value set of "key physical parameters" (KPPs) of particles from the "DATA BASE" subsystem, which stores data on the physical properties of particle materials (see Fig. 1). In addition, subsystem "SPLAT" allows you to determine the critical ranges boundaries of KPP values, within which the splat "model" shape remains inseparable – this is important for adjusting the technological regime for spraying coatings formed as a result of fixing splats on the surface during the spraying process [4-6]. The calculation of splat characteristics is based on theoretical self-similar solutions for the process of forming one splat and which have undergone experimental verification. Self-similar solutions require the so-

lution of a three-dimensional non-stationary boundary value problem with a free boundary for the Navier-Stokes equations. Solutions must be consistent with consistent with the equations of conjugate convective-conductive heat transfer and phase transformations in a spreading particle (in some cases, in the substrate) [4-6].

Subsystem “SPLAT” provides the opportunity for the subsystem “COATING” in the process of simulation the layered structure of the coating (at the stage of “laying splats” on the sprayed surface) to choose one of two model splat “morphologies” (Fig. 2): in the form of a disk and in the “smoothed” splat shape. In Fig. 2(b), the stepped profile of the smoothed splat shape is very noticeable, since of the three coordinates X, Y and Z, two coordinates X and Y take on discrete values with a given sampling step. The sampling step was deliberately chosen to be not small so that in Fig. 2(b) one could see the manifestation of the “stepping” of the splat profile [6].

Fig. 2. Microsections of model splat morphologies (black color – substrate; dark gray shade – splat core; light gray shade – peripheral annular splat part): (a) – disk (cylindrical splat); (b) – smoothed splat, equivalent in volume to disk splat [6].

The shape of the splat (selected from two possible ones) at the stage of laying the splat on the surface is deformed in accordance with the topography (relief) of the local area of the surface on which the splat is formed during spreading and solidification (Fig. 3). Based on the relief of the surface area, the trajectory and angle of the melt flow into the recess is determined in accordance with certain formulas [5]. All empirical parameters in these formulas were estimated at the stage of their calibration using experimental data.

The “COATING” subsystem [4-6] models the process of creating a coating layered structure in accordance with the *algorithm for sequential stochastic laying of splats* (essentially, the Monte Carlo method) on the sprayed surface. Different areas of the sprayed surface may differ in relief (see Figs. 3(a), (b)). The dimensions and shape of the splat are determined by the “SPLAT” subsystem (Fig. 2), and in the laying process of the splat, the “COATING” subsystem (more precisely, the laying algorithm) deforms the shape of the splat according to the relief (topology) of the contact surface area (Fig. 3).

(a) (b)

Fig. 3. Laying of the cylindrical splats (of gray shade) on a surface with a non-smoothed (variable) relief (black color): (a) – stepped relief; (b) – wave-shaped relief [6].

From Fig. 3(b) it follows that in the contact zone with the surface of the splat core, marked in dark gray in the figure on the right, pores are not formed due to significant discharge pressure when a drop of melt collides with the surface marked in black. Note that in Fig. 3(b) the right part of the splat periphery is not displayed, in contrast to the left part of the splat periphery shown in this figure, marked in a light gray shade (in the figure on the left). In addition, towards the periphery of the splat (in the figure on the left), the pores increase. It should be noted that the splat core radius R_{c0} is determined by the formula $R_{c0} \cong 1.1R_p$, where R_p is the radius of the particle in the form of a spherical drop of melt.

The absence of pores between the splat core and the substrate is ensured by the first algorithm of the splat laying procedure – *the algorithm "for recognizing and filling depressions on the surface in the contact zone with the splat core"* [6]. The second algorithm in the splat laying procedure is *the algorithm "for recognizing and filling recesses behind obstacles on the surface in the contact zone with the peripheral annular part of the splat"* [6]. Next, a *wave algorithm* [6] is used "*for scanning the sprayed surface with a non-smoothed (variable) relief"* to prepare an array of "support vertices" with subsequent approximation of the lower surface of the splat using B-spline surfaces [7].

The splat laying simulation procedure uses discretization with certain steps Δx and Δy (usually Δx=Δy) in the XY plane. Discretization is implemented in the form of a two-dimensional grid of nodes corresponding to the elements of a two-dimensional array of "support vertices" [6]. The elements of these array represent the z-coordinates of the "support vertices" of the sprayed surface in "floating point arithmetic" (no discretization on the Z axis). After the above-mentioned filling of the recesses, the "residual" volume of the liquid melt of the spreading drop allows us to finally adjust the thickness h_s of the splat.

Based on the array of "support vertices," the spline approximation determines the z-coordinates of the splat lower surface, corresponding to the relief of the sprayed surface. Using the adjusted splat thickness h_s for the selected splat morphology (Fig. 2), the z-coordinates of the splat upper surface are calculated (the reliefs of both surfaces of the splat are similar to each other, Fig. 3). Both arrays of the z-coordinates of the lower and upper surfaces of the splat, corresponding to the x- and y-coordinates of the nodal points of the partition grid are stored on the external disk into the corresponding files. Using this file, in the "Functional characteristics of coatings" subsystem, coating characteristics (such as porosity *P*%, roughness R_a, adhesive strength σ_{adg} of the coating to the base, etc.) are calculated.

3 Implementation of Program System for Parallel Running of SIMD-Tasks for Coating Simulation

3.1 Functionality of the Program System

As already mentioned in the introduction of the article, the creation of a program system with the ability to parallel execute SIMD-tasks is aimed at accelerating a series of simulations in which a certain class of coatings is modeled and their functional characteristics are calculated (porosity, strength of adhesion to the substrate, etc.).

The program system (PS) in terms of its functionality meets the following requirements:

- support for various formats for presenting and storing data;
- the ability to embed your own data presentation and storage formats;
- availability of a number of frequently used processing functions;
- the ability to create your own processing functions;
- the ability to develop, embed and execute various processing scenarios;
- convenient user interface with support for script debugging;
- display of processing results in a convenient form;
- system resistance to failures in processing functions;
- possibility of parallelization of calculations.

The PS implements the basic principle of optimal construction of software systems and complexes, which consists in creating several functional components (separate independent programs) interconnected by the ability to work with a common data storage (with files, databases, etc.). The PS structure is shown in Fig. 4.

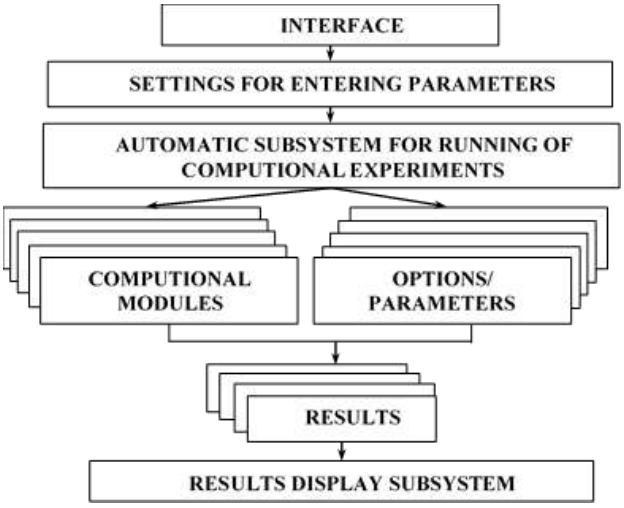

Fig. 4. Structure and composition of the PS.

The PS provides the following minimum set of components.

1. *Interface.* The main purpose of the interface is to enter initial data and parameters for executing a separate CE. The result of its work is a block of data of a certain structure, stored in a data warehouse, usually in the form of a specially designed file or record in a certain "database" (DB).

2. *Computing module (CM).* This program must access the data storage and find in it the corresponding "next" CE-block of input data corresponding to a certain coating simulation mode. Then the CM must perform basic calculations for simulating the coating with the specified parameters of the spraying mode and save the results in the storage in the form of another data block. In the introduction to the article, it was noted that all CMs are identical software copies (Fig. 4), implementing the computational basis of the program complex for coating simulation (Fig. 1). The need to reduce the time spent on carrying out (both a separate CE and the entire cycle of CEs) forces the creation of a CM architecture in the form of identical copies of CMs independently executed from each other (executed in parallel) on different computing nodes. Many copies of CMs distributed on different computers (or on nodes of a computing cluster) should be considered as a whole single program that allows you to simultaneously (in parallel) carry out a certain number of CEs (or the entire CE-cycle) depending on the computing power of the used multiprocessor computing system (MCS). With this organization of the PS, "parallelism of applications (tasks)" is performed, which determines the SIMD-architecture of the PS.

3. *Module for processing calculation results*. This program uses the results obtained from the CM and processes them in order to obtain "visual" data for a researcher in the field of creating gas-thermal coatings. It would seem that such programs simply need an interface, but this is not always the case. In most cases, it is enough for the user to provide ready-made report files (electronic reports), which can be used in further work. Examples of such files can be files with graphs, or tables, images, and sometimes full "high availability" reports with which the researcher (user) works. These "high availability" electronic reports may not be "tied" to the interface and modules listed above, and must be opened with standard software (for example, MS Office or other programs) available on any PC to ensure smooth data exchange.

4. *Scripts for automatically performing computational experiments*. This block of programs deals with dispatching processes, sequentially and repeatedly run copies of CMs with different sets of input data of the same structure and sizes (run SIMD-tasks), waiting for the completion of SIMD-tasks. In addition, this block controls the results processing module, which can be run either immediately after the completion of each CM-copy, or after the completion of all CM-copies. Then it provides the generation of a general electronic report, simplifying further access to the data.

The block of scripts, in accordance with specified criteria, has the ability to partially edit input data received from the interface program, which allows you to automate data entry by the operator, as well as eliminate his errors. Scripts for automatically performing computational experiments are used to control the resources of computing nodes and running such a number of CM-copies that optimally uses "critical" resources. In the case when the number of computing nodes is less than the total number of CEs,

each of the parallel running copies of the CM can execute several sequentially executed CEs.

The concept of experiment automation was a natural consequence of the development of coating simulation software [4-6]. This software allows you to calculate the functional and performance characteristics of powder coatings obtained by various gas-thermal technologies for spraying powder materials onto technical products (including APS, D-gun spraying and other methods). For a detailed study of the influence of various KPPs of sprayed particles and base (substrate) material on the characteristics of the coating, it was necessary to perform mass series of CEs.

Initially (before the development of the PS with an architecture for parallel running of similar SIMD-tasks), each CE was prepared manually: a set of parameters was specified for a specific CE through a graphical interface, then a calculation was carried out (lasting from several hours to several days). After completing the calculations of one CE, the next CE was again "manually" prepared and run for execution. Therefore, it was decided to move the sets of parameters into a separate configuration file and run the execution of all CEs in a special computing mode on a multiprocessor platform using the PS for parallel execution of SIMD-tasks.

The results of all CEs were saved to the PC hard drive. Further analysis of the results for each CE and their compilation into a general report "manually" sometimes led to errors. Therefore, it was decided to create a universal tabular report for each CE, including the KPPs of particles and substrate, which made it possible to further maintain a general log of all CEs, grouping them into series and recording time. Intermediate results reaching a volume of up to 20 GB for one CE are deleted after the completion of the report generation for each CE.

Detailed reports on the formation of coatings, as well as graphical versions of thin sections (vertical sections) of the coating, are of interest, but only if unexpected results are obtained as a result of the experiments. Despite the large volume of this data (about two gigabytes), it was decided to save the data on disk to restore the "evolutionary picture" of the experiments, including after a long time. To save disk space, software is used to reversibly compress information. Today, the volume of compressed results has already exceeded several terabytes, with an average compression ratio of ~80%, which suggests saving space on hard drives of at least ten terabytes.

Repeated modernization of the program complex for coating simulation gave rise to the problem of version control and changes, which they initially tried to solve using the traditional method, using the appropriate software (Hg Mercurial version control system). This made it possible to answer the question of exactly what changes were made, but did not allow us to compare the parameters and initial data of the CEs with the versions of the software package. Therefore, a rule was introduced: for each series of CEs, a separate current version of the source code of the software package is saved in order to subsequently track the changes made. Thus, the following algorithm was implemented as a set of scripts.

1. Initially, it is necessary to run the program and manually enter the parameters of the so-called "basic" CE spraying mode (technologically predictable spraying scenario).

2. Then the series name is assigned to the CEs series and the start date for the CEs series is indicated. Based on this, a separate directory is formed to store the results. A copy of the CM code is copied into the created directory, placed in the Src subdirectory and containing the basic parameter script.
3. In addition, many folders are created, the name of each of which contains a modified value of one of the KPPs, different from the value of this parameter from the "basic" set of KPPs (for example, Dp50μm - a changed value of 50 μm for the particle diameter D_p instead of the value of 30 μm from the base set). A copy of the CM is copied to each such folder, as well as a configuration file with the corrected value of a specific parameter (the remaining parameters repeat the corresponding parameters of the previous set of KPPs). The created set of folders is copied to the computing nodes (computers), then, using scripts, programs are run from the corresponding folders for each CE (for each computing node).
4. At the end of the calculations, temporary files are deleted, the report file of the CEs cycle is copied to a shared folder, adding the results to the common "report database".

3.2 Computational Tests for Determination of Optimal Loading Mode of Computing Nodes

To identify optimal loading modes for computing nodes, a series of computational tests were carried out. The same computational tests were performed on three computing systems (on three samples of computing nodes) and the execution time of test calculations was studied. In different tests, different numbers of CM-copies were run, but each time the same number of copies was run for each of the three systems (see Table 1).

Table 1 shows the following time parameters: Time_1 is the time of the main calculations for the specified number of CM-copies for each of the three systems; Time_2 is the time for processing and analyzing the results obtained after running of the CM-copies (also for each of the three systems). The following computer system configurations (the samples of computing nodes) were used for testing:

- **System 1**: Inteli7-4710MQ (2.5GHz): 4 cores, 8 computing threads, 8 GB RAM, Win7x64, SSD: KingstonSV300S37A240G (240 GB, communication speed 450 MB/s);
- **System 2**: Inteli5-4690 (3.5 GHz): 4 cores, 4 computing threads, 12 GB RAM, Win7x64, HDD: ST3500630AS (500 GB, spindle speed7200 rpm);
- **System 3**: Inteli5-4690 (3.5 GHz): 4 cores, 4 computing threads, 12 GB RAM, Win7x64, SSD: Corsair Force GS (256 GB, communication speed 500 MB/s).

As can be seen from Table 1, the optimal mode for each of the three systems is the use of 4 parallel computing processes (based on the time spent on executing one copy).

Table 1. Running time for multiple CM-copies on three computing systems.

Number of running CM-copies	Running time (in hours): Time_1 + Time_2 = Total time		
	System 1	**System 2**	**System 3**
1	3.3+1.1=4.4	4.0+1.5=5.5	3.6+1.2=4.8
2	5.6+1.9=7.5	6.5+2.7=9.2	6.0+2.1=8.1
3	6.1+2.5=8.6	7.3+3.4=10.7	6,8+2.7=9.5
4	7.0+1.6=8.6	7.9+2.1=10.0	7.6+1.7=9.3

The performance of each of the 3 systems was limited by hard drives. Therefore, CMs were run on high-speed hard drives in further running CEs. When distributing the load on computing nodes with different performance, the peculiarities of the influence of the parameter values of the initial sprayed particles on the coating calculation time were taken into account. The implemented architecture of the PS makes it possible to carry out parallel running CEs over a long period of time (in round-the-clock operation for several weeks). Upon completion of the work, a general electronic report is generated, which is duplicated in the archive.

4 Using a Program System with an Architecture for Parallel Running of Similar SIMD-Tasks for Coating Simulation

Analyzing the simulation results of coatings made of titanium nickelide (TiNi), taking into account various sets of KPPs characterizing different modes of coating spraying, it can be stated that the following functional characteristics (properties) of coatings change significantly: R_a – coating roughness; P% – coating porosity; σ_{adg} – strength of adhesion of the coating to the substrate.

The main results of the CEs at the stage of modeling coatings (with thickness H = 100 μm) are summarized in Tables 2-9, in which, similarly to work [8], in addition to the relative adhesive strength of coatings $\overline{\sigma}_{adg}$, coating roughness R_a and coating porosity P%, the powder particle KPPs and calculated splat parameters are given. Similarly to work [8], in Tables 2-9 the following designations of quantities are used: T_p – particle temperature; U_p – particle velocity; D_p – particle diameter; T_b – base (substrate) temperature; D_s – splat diameter; h_s – splat height (thickness at its center).

Similarly to work [8], the value $\overline{D}_s$ is normalized value of the splat diameter D_s, expressed in relative units (r.u.) and which is otherwise called the "spreading factor" of the melt particle ($\overline{D}_s = D_s / D_p$). The value $\overline{h}_s$ is the normalized value of the splat thickness h_s, i.e. $\overline{h}_s = h_s / D_p$. The value $\overline{\sigma}_{adg}$ determines the relative strength of adhesion of the coating to the base (more precisely, of the first monolayer of the coating to the substrate). In other words, it determines the ratio of the absolute adhesive strength of the coating to the tensile strength (i.e., it determines the proportion of the maximum possible adhesive strength). Similarly to work [8], the temperature T_c determines the contact temperature at the point of collision of the melt droplet with the surface (with

the substrate). The integer value of the "Scenario" parameter indicates the number of the scenario of the melt droplet spreading on the substrate (see below) [8, 9]:

1. spreading and simultaneous solidification of the droplet on the solid base;
2. spreading and simultaneous solidification of the droplet, and local submelting of the base at the contact spot with the droplet;
3. spreading of the droplet over the solid base surface, and subsequent cooling and solidification of the spread layer;
4. spreading of the droplet accompanied with simultaneous local submelting of the base, followed by subsequent cooling and solidification of both.

Let's analyze Tables 2-9, in which, based on the results of the CEs, the calculated splat parameters and functional characteristics of TiNi coatings on steel (Steel45) and titanium (Ti) substrates are entered.

Table 2. Calculated splat parameters and functional characteristics of TiNi coatings on a Steel45 substrate when changing the temperature parameter T_p of the particles and maintaining the conditions: U_p = 200 m/s, D_p = 30 μm, T_b = 400 K.

T_p, K	D_s, μm	$\overline{D_s}$, r.u.	h_s, μm	$\overline{h_s}$, r.u.	R_a, μm	P%	$\overline{\sigma}_{adg}$, r.u.	T_c, K	Scenario
1600	119	3.950	1.28	0.043	1.98	3.998	0.0257	1222.4	1
1650	121	4.038	1.23	0.041	1.92	3.936	0.0431	1256.7	1
1700	150	5.002	0.81	0.027	2.09	3.942	0.0967	1291.0	1
1750	201	6.701	0.45	0.015	2.05	4.239	0.1521	1325.2	3
1800	201	6.701	0.45	0.015	1.99	4.009	0.1997	1359.5	3
1850	201	6.701	0.45	0.015	2.04	3.981	0.2475	1393.8	3

Table 3. Calculated splat parameters and functional characteristics of TiNi coatings on a Steel45 substrate when changing the velocity parameter U_p of the particles and maintaining the conditions: T_p = 1600 K, D_p = 30 μm, T_b = 400 K.

U_p, m/s	D_s, μm	$\overline{D_s}$, r.u.	h_s, μm	$\overline{h_s}$, r.u.	R_a, μm	P%,	$\overline{\sigma}_{adg}$, r.u.	T_c, K	Scenario
100	100	3.337	1.80	0.060	1.63	11.513	0.0238	1122.0	1
150	110	3.682	1.48	0.049	1.56	10.184	0.0242	1122.0	1
200	119	3.950	1.28	0.043	1.98	3.998	0.0257	1222.4	1
250	210	7.007	0.41	0.014	2.34	1.685	0.0261	1222.4	3
300	218	7.267	0.38	0.013	2.10	0.690	0.0280	1222.4	3
350	225	7.494	0.36	0.012	0.48	0.766	0.0277	1222.4	3
400	231	7.697	0.34	0.011	0.46	0.896	0.0245	1222.4	3

Table 4. Calculated splat parameters and functional characteristics of TiNi coatings on a Steel45 substrate when changing the diameter parameter D_p of the particles and maintaining the conditions: T_p = 1600 K, U_p = 200 m/s, T_b = 400 K.

D_p, μm	D_s, μm	$\overline{D}_s$, r.u.	h_s, μm	$\overline{h}_s$, r.u.	R_a, μm	P%,	$\overline{\sigma}_{adg}$, r.u.	T_c, K	Scenario
20	72	3.578	1.04	0.052	1.21	3.432	0.0179	1122.0	1
30	119	3.950	1.28	0.043	1.98	3.998	0.0257	1222.4	3
40	284	7.098	0.53	0.013	2.13	4.529	0.0446	1222.4	3
50	371	7.422	0.61	0.012	2.62	5.070	0.0627	1222.4	3
60	462	7.697	0.68	0.011	3.89	5.851	0.0822	1222.4	3
70	556	7.938	0.74	0.011	7.12	8.283	0.0994	1222.4	3
80	652	8.153	0.80	0.010	8.46	10.422	0.1191	1222.4	3
90	751	8.347	0.86	0.010	12.24	13.526	0.1402	1222.4	3
100	853	8.525	0.92	0.009	15.07	16.667	0.1577	1222.4	3

Table 5. Calculated splat parameters and functional characteristics of TiNi coatings on a Steel45 substrate when changing the base (substrate) temperature parameter T_b and maintaining the conditions: T_p = 1600 K, U_p = 200 m/s, D_p = 30 μm.

T_b, K	D_s, μm	$\overline{D}_s$, r.u.	h_s, μm	$\overline{h}_s$, r.u.	R_a, μm	P%,	$\overline{\sigma}_{adg}$, r.u.	T_c, K	Scenario
300	116	3.852	1.35	0.045	1.97	3.912	0.0148	1191.0	1
400	119	3.950	1.28	0.043	1.98	3.998	0.0257	1222.4	1
500	122	4.061	1.21	0.040	2.05	4.126	0.0450	1253.9	1

Table 6. Calculated splat parameters and functional characteristics of TiNi coatings on a titanium substrate when changing the temperature parameter T_p of the particles and maintaining the conditions: U_p = 200 m/s, D_p = 30 μm, T_b = 400 K.

T_p, K	D_s, μm	$\overline{D}_s$, r.u.	h_s, μm	$\overline{h}_s$, r.u.	R_a, μm	P%,	$\overline{\sigma}_{adg}$, r.u.	T_c, K	Scenario
1600	201	6.701	0.45	0.015	1.72	3.880	0.0006	1222.4	3
1650	201	6.701	0.45	0.015	1.90	4.030	0.0011	1256.7	3
1700	201	6.701	0.45	0.015	1.96	4.148	0.0020	1291.0	3
1750	201	6.701	0.45	0.015	2.05	3.984	0.0029	1325.2	3
1800	201	6.701	0.45	0.015	1.89	4.022	0.0048	1359.5	3
1850	201	6.701	0.45	0.015	2.00	4.244	0.0078	1393.8	3

Table 7. Calculated splat parameters and functional characteristics of TiNi coatings on a titanium substrate when changing the velocity parameter U_p of the particles and maintaining the conditions: T_p = 1600 K, D_p = 30 μm, T_b = 400 K.

U_p, m/s	D_s, μm	$\overline{D}_s$, r.u.	h_s, μm	$\overline{h}_s$, r.u.	R_a, μm	P%,	$\overline{\sigma}_{adg}$, r.u.	T_c, K	Scenario
100	111	3.705	1.46	0.049	1.76	11.606	0.0002	1122.0	1
150	190	6.326	0.50	0.017	1.83	10.423	0.0009	1122.0	3
200	201	6.701	0.45	0.015	1.72	3.880	0.0006	1222.4	3
250	210	7.007	0.41	0.014	2.32	1.652	0.0005	1222.4	3
300	218	7.267	0.38	0.013	2.19	0.728	0.0004	1222.4	3
350	225	7.494	0.36	0.012	0.42	0.774	0.0004	1222.4	3
400	231	7.697	0.34	0.011	0.45	0.895	0.0003	1222.4	3

Table 8. Calculated splat parameters and functional characteristics of TiNi coatings on a titanium substrate when changing the diameter parameter D_p of the particles and maintaining the conditions: T_p = 1600 K, U_p = 200 m/s, T_b = 400 K.

D_p, μm	D_s, μm	$\overline{D}_s$, r.u.	h_s, μm	$\overline{h}_s$, r.u.	R_a, μm	P%,	$\overline{\sigma}_{adg}$, r.u.	T_c, K	Scenario
20	79	3.974	0.84	0.042	1.31	3.414	0.00006	1122.0	1
30	201	6.701	0.45	0.015	1.72	3.880	0.00057	1222.4	3
40	284	7.098	0.53	0.013	2.20	4.665	0.00086	1222.4	3
50	371	7.422	0.61	0.012	3.11	5.019	0.00124	1222.4	3
60	462	7.697	0.68	0.011	4.09	6.047	0.0010	1222.4	3
70	556	7.938	0.74	0.011	7.81	8.859	0.0011	1222.4	3
80	652	8.153	0.80	0.010	8.30	10.399	0.0017	1222.4	3
90	751	8.347	0.86	0.010	11.83	14.143	0.0019	1222.4	3
100	853	8.525	0.92	0.009	14.51	17.110	0.0018	1222.4	3

Table 9. Calculated splat parameters and functional characteristics of TiNi coatings on a titanium substrate when changing the base (substrate) temperature parameter T_b and maintaining the conditions: T_p = 1600 K, U_p = 200 m/s, D_p = 30 μm.

T_b, K	D_s, μm	$\overline{D}_s$, r.u.	h_s, μm	$\overline{h}_s$, r.u.	R_a, μm	P%,	$\overline{\sigma}_{adg}$, r.u.	T_c, K	Scenario
300	201	6.701	0.45	0.015	2.01	3.964	0.00032	1191.0	3
400	201	6.701	0.45	0.015	1.72	3.880	0.00057	1222.4	3
500	201	6.701	0.45	0.015	1.93	4.006	0.00099	1253.9	3

The value $\overline{D}_s$ (spreading factor) for splats from metal [10] must satisfy the condition $\overline{D}_s < 4.5$ (starting from a value of 5, breaks appear on the circular periphery of the splat). As can be seen from Tables 2-9, this condition is satisfied by scenario 1, and scenario 3 is not satisfactory. When spraying TiNi particles onto a titanium substrate, only scenario 3 is practically realized, with the exception of the technological spraying

mode (scenario 1, $\overline{D_s} < 4.5$): T_p = 1600 K, U_p = 100 m/s, D_p = 20 μm, T_b = 400 K. Therefore, from a technological point of view, spraying coatings of titanium nickelide particles onto a steel substrate deserves more attention. The technological mode of spraying coatings of TiNi particles onto a Steel45 substrate corresponds to wider ranges of KPPs, namely: T_p = 1600-1700 K, U_p = 100-200 m/s, D_p = 20-30 μm, T_b = 300-500 K.

It is known [11] that with increasing particle temperature T_p, and consequently with increasing contact temperature T_c, the relative adhesive strength $\bar{\sigma}_{adg}$ initially increases rapidly, and then the increase slows down (and may approach 1). The above mentioned growth trend of $\bar{\sigma}_{adg}$ is conformed in Table 2. The contact temperature T_c also increases with increasing substrate temperature T_b (see Table 5), therefore the relative adhesive strength $\bar{\sigma}_{adg}$ also increases (up to approximately 0.045). However, as the particle temperature T_p increases, the relative adhesive strength $\bar{\sigma}_{adg}$ reaches a higher value of 0.2475.

As can be seen from Table 4, with increasing diameter D_p of particles, the value $\bar{\sigma}_{adg}$ also increases (to a value of 0.1577), giving way to growth of $\bar{\sigma}_{adg}$ with increasing of T_p.

According to the conclusions given in [11], the relative adhesive strength $\bar{\sigma}_{adg}$ in theoretical terms does not change when the velocity of particles changes (see Table 3).

From Table 2 it follows that for an acceptable technological mode with the highest value $\bar{\sigma}_{adg}$ = 0.0967 can be corresponded the mode with the parameters: T_p = 1700 K, U_p = 200 m/s, D_p = 30 μm, T_b = 400 K. Table 5 indicates an increase of $\bar{\sigma}_{adg}$ of approximately 1.751 times as the substrate temperature increases from 400 to 500 K (while maintaining scenario 1 and $\overline{D_s} < 4.5$). Therefore, we can consider the optimal technological spraying mode to be the one with the following parameters: T_p = 1700 K, U_p = 200 m/s, D_p = 30 μm, T_b = 500 K, for which the estimate $\bar{\sigma}_{adg}$ will increase by 1.751 times, i.e. $\bar{\sigma}_{adg} \cong 0.17$.

In [12 - 14] for titanium nickelide (B2-phase of TiNi) data are given on the tensile strength (denoted as σ_{ts}). In [12] states that the presence of phase precipitates Ti_2Ni and $TiNi_3$ in the B2-phase matrix of TiNi, even with small concentrations, leads to exceeding the tensile strength value of 950-1000 MPa, which characterizes the minimum value σ_{ts} for the B2-phase of TiNi. In [13] a high tensile strength value of 1885 MPa was achieved for wire made of nanostructured titanium nickelide, taking into account multiple compression by drawing and controlled multi-stage heat treatment. In [14] on page 21 indicates that with a certain chemical composition of titanium nickelide, as well as during thermomechanical processing, the tensile strength can reach values of up to 2000 MPa. A value of 1885 MPa can be taken as the base value for the B2-phase of TiNi.

The "absolute" adhesive strength σ_{adg} is determined by multiplying the relative adhesive strength $\bar{\sigma}_{adg}$ by the "tensile" strength value σ_{ts}, i.e. [11]

$$\sigma_{adg} = \bar{\sigma}_{adg} \cdot \sigma_{ts} .$$

Using the more likely value range of 1885-2000 MPa, corresponding to the σ_{ts}-values (values decreasing towards 1000 MPa are unlikely) and the estimate $\bar{\sigma}_{adg} = 0.17$ (obtained above), the absolute adhesive strength values for TiNi coatings range from 320 to 340 MPa (a range 170 - 320 MPa is unlikely). We can say that the obtained estimates of the expected range of adhesive strength for TiNi coatings on a steel substrate are quite high.

For acceptable spraying modes, in particular for the optimal technological mode (T_p = 1700 K, U_p = 200 m/s, D_p = 30 μm, T_b = 500 K), the roughness R_a is quite small (about 2 μm) and is less than for many other coatings [15]. Its share in relation to the thickness of the coatings (H = 100 μm) is about 2%.

Analyzing the porosity of TiNi coatings on both steel and titanium substrates, we can say that the porosity P% of the coatings practically varies little when the particle temperature T_p changes within 250 K (see Tables 2 and 6). The porosity of TiNi coatings also varies little for both types of substrate and with changes in substrate temperature T_b (see tables 5 and 9). Depending on the increase in particle diameter D_p (Tables 4 and 8), porosity increases significantly (close to a linear trend), which is typical for many metal coatings. But within the range of changes in particle diameter up to 70 μm (see Tables 4 and 8), porosity remains within the range of 4 to 8%, traditional for metal coatings in the case of APS. The particle velocity for the APS spraying mode is in the range of 200-300 m/s. An expected fact is that porosity tends to decrease with increasing particle velocity (see Tables 3 and 7). Starting from values of 300 m/s and higher (for example, for D-gun spraying and HVOF technologies), the porosity decreases sharply and becomes less than 1%, thereby realizing very dense coatings that are in demand in the materials industry [16-20].

5 Conclusions

Summarizing the results of computational experiments, we can say that the adhesive strength of TiNi coatings is quite high and practically does not depend on particle velocity. In plasma spraying mode (APS), the porosity of coatings does not exceed traditional values (up to 7-8%), and for D-gun spraying and HVOF – less than 1%. The roughness of TiNi coatings is quite small and does not exceed 2 μm. Such very dense coatings with low roughness are in demand in the materials industry [16-20]. Formulating conclusions regarding the created modeling software, we can say the following.

The implemented program system, despite its simplicity, provides a number of significant advantages:

– there is no need to parallelize each copy of the CM;

- systematization of the obtained CE-results is carried out, the ability to quickly create a general electronic report with illustrative research material;
- saving time by automating the preparation of a general electronic report (instead of the work of the researcher to compile the report "manually");
- the CEs cycle is carried out in a "conveyor" way and there is no loss of time between the execution of individual CEs;
- errors arising due to the so-called "human factor" are practically eliminated;
- a compact archive is created that makes it possible to obtain comprehensive data about each CE after a long time, which fully justifies the time spent on developing the corresponding software modules.

This technique has been tested and is recommended for embedding into computer programs that perform a series of similar calculations.

Acknowledgments

This study was supported by the Basic Research Program of the State Academies of Sciences for 2021–2023, project no. AAAA-A17-117030610124-0. This study was performed on the equipment of the Collective Use Center Mechanics (Khristianovich Institute of Theoretical and Applied Mechanics of the Siberian Branch of the Russian Academy of Sciences).

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