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# PHENOMENOLOGICAL MODELING OF VOLUME NANOMATERIALS WITH FORM MEMORY

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*The paper presents a phenomenological approach to modeling bulk memory nanomaterials form. A phenomenological model has been proposed that can be applied to model the behavior of nanomaterials with shape memory properties. The study of shape memory alloys as functionally inhomogeneous materials with the properties of pseudo-elastic-plasticity is presented. The phenomenological model is confirmed by experimental data. Tables of diagrams for different temperatures of alloys with shape memory are given.*

*Key words: modeling, functionally inhomogeneous materials, nanomaterials, phenomenological approach, large deformations*

**Problem statement.** In recent decades, nanotechnology has become a strategic industrial direction in the world and in Ukraine. There is a great interest in materials with nanostructure in connection with the real possibility of practical implementation of their unique properties in various fields of science and technology. Many countries around the world conduct research and development in the field of nanotechnology and Ukraine has its own national programs in this area. Intensive scientific work in the field of nanotechnology is characterized by an exponential growth of scientific publications [1].

In recent years, for the first time, the principles of creating nanostructured states in bulk metallic materials with shape memory effects, which allow to change their structural and functional properties at a qualitatively new level, have been formulated, thoroughly researched and brought to practical testing. Works on creation of scientific bases of reception of volume nanostructured metal materials, development and introduction of their highly effective nanotechnologies improving quality and a complex of properties of materials with shape memory, have priority character, differ in the fundamental novelty, originality of theoretical and technological approaches and decisions. high efficiency. As a result of systematic research, the effect of simultaneous increase in strength and ductility of practically important for engineering and medicine alloys with shape memory based on nickel titanium was revealed and explained [1].

It is shown that in bulk nanomaterials record high values of strength (up to 3.0 GPa), fluidity (up to 2.5 GPa), elongation (up to 80%), relative narrowing (up to 70%) can be achieved simultaneously. reverse deformation (9 ... 15%), reactive stress (up to 2.0 GPa) in the implementation of 100% of the shape memory in a narrow temperature range. The nature of the effect, its physical conditions and structural mechanisms, the influence of doping, phase composition and structure-forming external influences are established. A number of developed methods of strengthening are patented [1].

Controlled doping of alloys based on TiNi, which allows to regulate their stability with respect to decay and MP, the use of various methods of thermal and thermomechanical treatment provided a very effective targeted change in their structure and physical and mechanical properties and opened new unique opportunities to change microstructure, influence on phase transformations and related physical and mechanical properties of TiNi-based alloys.

Such basic characteristics make it possible to widely use these materials in various fields of science and technology.

Depending on the microstructure, bulk nanomaterials have different properties, including the shape memory property. Bulk nanomaterials with shape memory properties can be considered as functionally inhomogeneous materials with pseudo-elastic-plasticity.

Pseudo-elastic-plasticity is the ability of a material under active load to accumulate deformations of a certain value in the mode of higher temperature, and then after unloading (through the hysteresis loop) to return to the initial state. The main mechanism is the inverse martensitic transformation between the phases of the solid, which can occur at room temperature. Such a transformation can be caused by a change in temperature or by force factors. The material is also characterized by nonlinear mechanical behavior and large deformations. Alloys that show shape memory and pseudo-elastic-plasticity are: NiTiAuCd, CuAlNi, CuSn, CuZn, NiFeGa, NiTiNb, NiNiGa, NiFeGa, NiPi, NiPeGa, NiPiGi [2; 3]. Such characteristics make SPF suitable for use in various devices or as components in some advanced composite materials. NiTi alloy leads in most such applications due to its structural properties.

The first shape memory alloys (SPFs) were developed in the middle of the last century; however, there are no rigorous and reliable fixed-level defining models required for the engineering applications of these materials.

The relationship between microscopic and macroscopic behavior is very complex and has not yet been developed to the extent required by such models and practical tasks. This is partly due to the strong dependence of mechanical reactions on temperature, load velocity, deformation range, geometry of the body under study, thermomechanical history and nature of the environment, as well as the interaction between these parameters.

The analysis shows that there are currently a number of models for describing the thermomechanical behavior of alloys with shape memory, pseudo-elasticity and pseudo-elastic-plasticity. Most of them are based on classical ideas, ie aim to directly describe the experimental data obtained on different samples under simple and complex loads. However, as established in experimental studies, the behavior of the material at the point of the body in the General case differs from the behavior of the sample as a whole and there may be significant deformations.

The main task of the nonstationary theory of thermoplasticity is to determine the velocities and components of stress and strain tensors that occur in a three-dimensional body during its loading and heating, when some elements of the body work beyond the elasticity of the material. The process of loading will be considered as changing over time, which can cause movement of certain parts of the body.

First, the isotropic and homogeneous three-dimensional body V, bounded by the surface S, at the initial time *t = 0* is in a natural unstressed state at a temperature $T_0(\theta_i),\ i = 1;2;3.$ Then the body is heated and loaded by external forces. These can be three-dimensional forces that affect each element of the body. Surface forces acting on one part of the body surface. On the second part of the surface of the body, which can be fixed in some way, the velocities are set as a function of coordinates and time.

Suppose that the heating and loading of the body occur so that there are deformations that can significantly affect the temperature change of this element. We will consider such loading processes and temperature levels at which the rheological properties of the material are not detected. The configuration of a body is given by the equation of the surface that limits it. In addition, you need to specify the thermophysical and mechanical characteristics of the body material and the conditions of its heat exchange with the environment.

Thermophysical properties of the material are characterized by coefficients of thermal conductivity and thermal conductivity, which may depend on temperature. The heat transfer conditions are set in the form of appropriate boundary conditions, and the mechanical characteristics of the material in the study of deformation processes on straight trajectories and the trajectory of small curvature are set in the form of instantaneous tensile diagrams of samples obtained at different fixed temperatures. In addition, the values of the Poisson's ratios $\nu$ and linear thermal expansion are set.

Based on these data, it is necessary to determine the temperature, the three components of the velocity vector, the six components of the stress tensor and the six components of the strain tensor. Therefore, it is necessary to determine sixteen unknown functions of time and three coordinates. To do this, use the equations of motion, geometric and physical equations, as well as the equation of thermal conductivity. The temperature field at any point in the body in the presence of heat sources and in the case of heat, which is released during its deformation, is determined by solving the equation of thermal conductivity under certain initial and boundary conditions [2, 3].

After determining the temperature field for different points in time, the components of the velocity vector and the components of stress and strain tensors satisfying three differential equations of motion, six geometric equations and six physical equations are searched. These equations are solved under certain initial and boundary conditions. The initial conditions are set for all unknowns at the initial time. On the part of the body surface where the given forces *b(xi, t)*, the components of the stress tensor must satisfy three boundary conditions:

$$\sigma_{in}(\alpha_k,t)=\sigma_{ij}\cdot n_j,\quad i,j,k=1,2,3$$ ,

where $n_j$ are the directing cosines of the external normal to the body surface at the corresponding point. On the other part of the surface, where the specified components of the velocity vector, the velocity must take the specified values:

$$v_i=V_i(x_j,t)$$

Another formulation of boundary conditions is possible when three conditions are taken on the surface of the body, taken in a certain way from the above conditions.

The definition of the unknown will be found as follows. The main unknowns are three components of the velocity vector and six components of the stress tensor, for which the boundary conditions are directly formulated. In this case, all components of the strain tensor are excluded from the six physical equations by means of geometrically nonlinear Cauchy relations, which are then determined on the basis of already known components of the velocity vector.

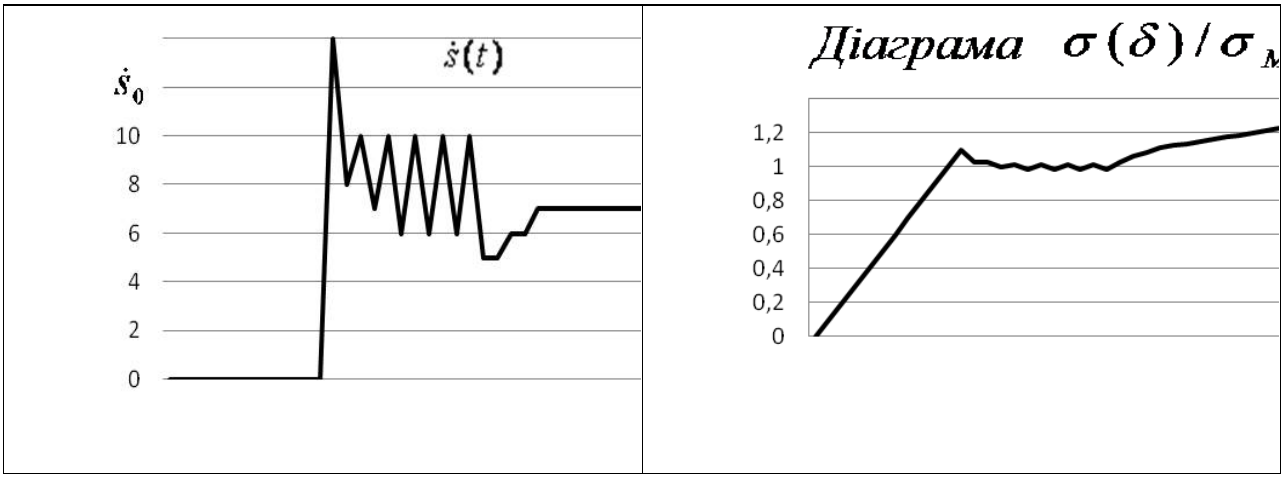
When solving the nonstationary thermoplasticity problem, we will use the defining equations that describe nonisothermal loading processes along both rectilinear trajectories and small curvature deformation trajectories. After completing the task on the geometry of the deformation trajectory, it is possible to draw a conclusion about the reliability of the used determining relations.

**Solving the problem.**

Currently, a number of models are known to describe the thermomechanical behavior of shape memory alloys. Most of them are based on classical phenomena, ie they aim to directly describe the experimental data obtained on different macro samples under simple and complex load. However, as established in experimental studies, the behavior of the material at a point on the body in the general case differs from the behavior of the sample as a whole. We formulate the properties of the phenomenological model used to describe the behavior of bodies made of pseudo-elastic-plastic materials. Deformation at a point is represented as the sum of the elastic component; jump of deformation at phase transition; plastic deformation, which is subject to the theory of flow with kinematic and translational strengthening; deformation caused by temperature changes. It is assumed that the properties of the material depend on the temperature.

To describe the elastic deformation and the deformation of the phase transformation, we use a diagram of an elastic material consisting of three curvilinear or rectilinear sections. This interpretation leads to an unstable stress-strain diagram, and to describe the thermomechanical behavior of samples of different shapes, it is necessary to have a solution of the boundary value problem taking into account the development of the phase transformation deformation front. In this case, we will take into account not only the ambient temperature, but also the heat released during the phase transition. This interpretation allowed us to propose a model from a single position and describe a number of experimental data on different samples under different loading conditions, including cyclic temperature and force. Specific dependences for mechanical parameters are established. It is shown that the phase separation boundary moves at a constant speed for the selected temperature. It is established that classical material diagrams are a curve that envelops a family of material diagrams at a point, which is constructed for certain laws of change of the velocity of the deformation rupture front [4].

The results of the calculations are given below. Figure 1 shows a typical dependence for the rate of propagation of the phase transition over time. Its schedule has three sections. In the first section, the speed is zero, and in the third reaches a constant value. Between them is a section with variable speed. As a result of calculating the tangent module at each step of integration over time for the integrated diagram of the material, we also have three characteristic sections.




1 a) 1 `b)

**Figure 1. Phase transition velocity (1 a) and integrated material diagram (1 b).**

The first section corresponds to the elastic behavior of the material. The third characterizes the strengthening of the material. Between them is a section that resembles the behavior of a perfectly plastic material. Similar areas occur during unloading, but at certain temperatures.

**Experimental substantiation of the model.**

This section is devoted to the experimental substantiation of the variant of the proposed model of material behavior with shape memory and thermo-pseudo-elastic-plasticity. The model provides the possibility of quantitative estimation of the complex interaction between stress, temperature, deformation, sample loading rate and heat released in the process of passing the front of phase transformations along the sample.

Thus, the mechanical characteristics of the material in the study of deformation processes are set in the form of instantaneous tensile diagrams of the samples, which are obtained at different values of temperature, and, if necessary, allow you to build an integrated diagram of the material.

Processing of experimental data of work [5] allowed to build tables and diagrams for different values of temperature (respectively 100, 90, 80, 70, 60, 50, 40, 30, 20, 10, 0 degrees Celsius). The results of the comparison with the experimental data are partially given below in the form of diagrams. The upper lines (σ>…) correspond to the active load of the sample, and the lower (σ <…) - unloading at a certain temperature.

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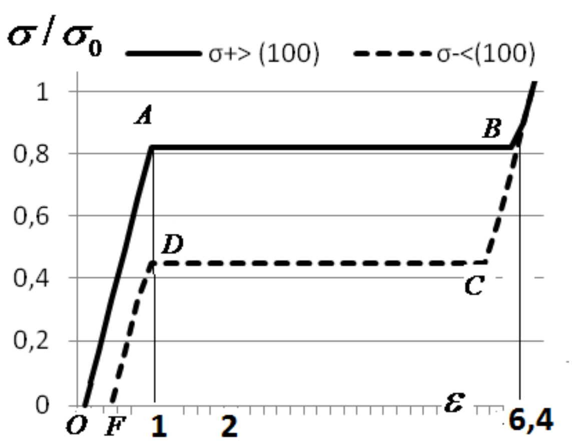
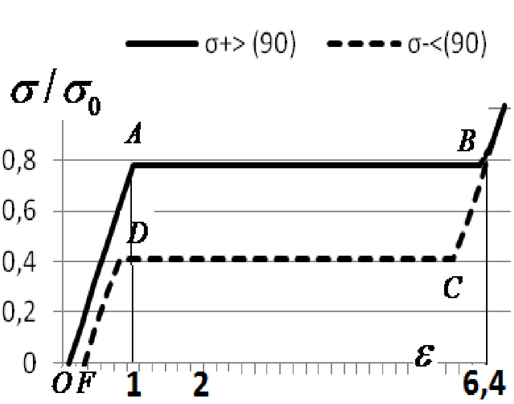
Note that the diagrams shown in Figures 3 are constructed for fixed values of temperature without taking into account the heat released during the phase transformation at the material point.




2 a)

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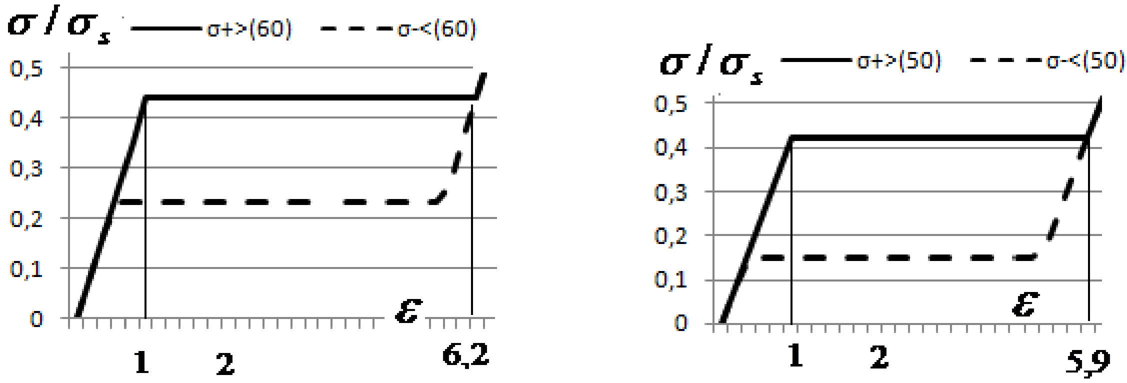
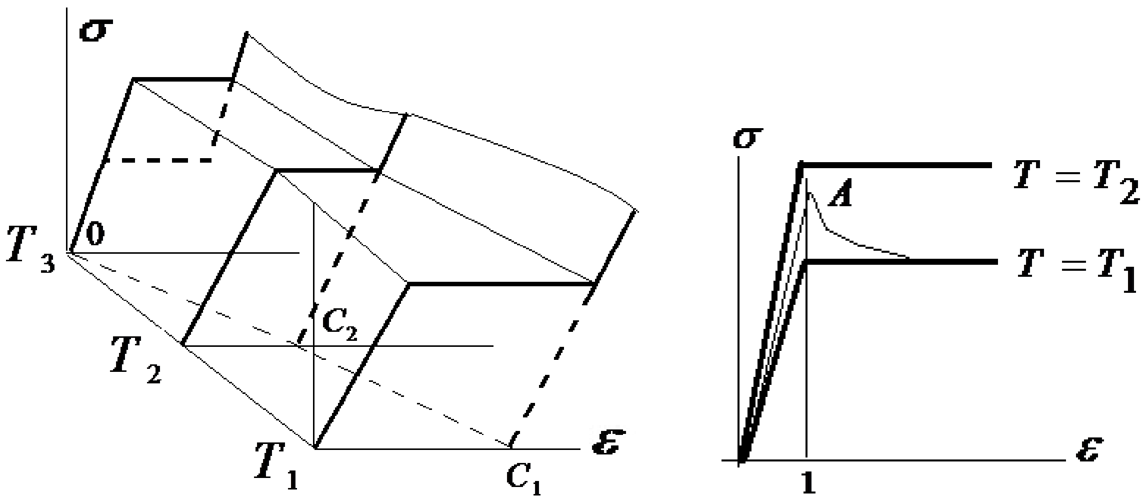



2 c) 2 g)

**Figure 2. Local diagrams of the material at 100 0 C (3 a), 90 0C (3 b), 60 0C (3 c), 50 0C (3 g).**

The refined phenomenological model of the behavior of the alloy at the material point is based on the above results. Graphically, it differs from the previous model by the presence of a flow tooth at the boundary of the elastic section under active loading and a smooth transition of the aircraft in the CD during unloading. The corresponding qualitative results are shown in Figure 3.




3 a) 3 b)

**Figure 3. Local diagram of the material.**

Note that the diagram for the refined phenomenological model (Figure 3 b)) is constructed for the same initial temperature as the diagram shown in Figure 3 a). The size of the fluidity tooth is modeled separately and compared with experimental data. It is necessary to solve the equation of thermal conductivity separately and determine the additional values of deformation and stress by the temperature difference [3]. In fact, the diagram with the fluidity tooth is a projection of the trajectory that goes along the instantaneous thermo-mechanical surface.

To obtain the calculation formulas of the refined model, an auxiliary problem related to the construction of an instantaneous thermo-mechanical surface was considered. Suppose that in three-dimensional $\varepsilon, T, \sigma$ space the coordinates of four points are given $P_i(\varepsilon_i, T_i, \sigma_i), i = 1; 2; 3; 4.$ The equation of the thermomechanical surface passing through these points is written as follows:

$$\sigma = a\varepsilon + bT + c\varepsilon T + d. \quad (1)$$

Unknown coefficients $a, b, c, d$ are searched for from a system built on the basis of this expression for a given four points $P_i$ of an instantaneous thermo-mechanical surface. After their calculation, you can build such a surface on two adjacent diagrams obtained for $T = T_1$ and $T = T_2$, on the interval $T \in [T_1; T_2]$. Under active load, the total thermo-mechanical surface consists of three separate surfaces. This is the surface for the elastic part, the surface where the jump deformations caused by phase transformation and the plastic part of the surface. The thermo-mechanical surface is similarly modeled and at unloading.

Thus, having a thermo-mechanical surface and the law according to which the temperature changes at one or another point of the sample, it is possible to refine the local diagram of the material.

**Conclusions:** The paper proposes a phenomenological approach to the modeling of bulk nanomaterials, if we consider them as functionally inhomogeneous materials with the property of pseudo-elastic-plasticity. The proposed approach can be used in terms of macro-level.

The paper proposes a phenomenological model and provides theoretical studies of alloys with shape memory.

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