Nanomechanics and its applications: mechanical properties of materials

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Abstract - **In this work has described a methodology of the using of Nanomechanics in practice. On the basis of Nanomechanics principles, the potential force field in nanostructure is investigated here. The nanostructures of the materials are described and the differential equations of the mechanical motion of nanoparticles in potential force field are written and have been solved the using of the Lennard-Jones's potential. The theoretical expressions of the modulus of elasticity of materials are deduced and have been constructed corresponding diagrams for practical usage. The method for definition of mechanical properties of materials in nano-dimensional level is developed.**

Keywords: **Nanomechanics, Mechanical system, Equation of motion, Lennard-Jones potential, Crystal lattices, Mechanical properties of materials.**

I. Introduction

Nanomechanics is the perfect tool to study and to improve the mechanical properties (stiffness, strength, flexibility, plasticity) of the machine parts materials. Nanomechanics also is the new instrument for filling an emptiness between quantum mechanics which deals with the movement of atoms and molecules and the classical mechanics. Here the researches are conducted theoretically and experimentally which are the indifference of Theoretical Mechanics. Entering a new phase of development, many concepts and terms of the Theoretical and Applied Mechanics are significantly different from its original form and content in recent years. The new branch of Mechanics - Nanomechanics is the scientific basis of mechanical studying and control of nanostructures. It is a new theoretical base for tribology, i.e. a new object of friction and wear of machine elements. The machines and mechanisms installed on the basis of the principles of Nanomechanics which established will be expected to increase their longevity and accuracy in 10-15 times in the near future. Nanomechanics is the multidisciplinary science between Quantum mechanics, Theoretical mechanics, Fluid mechanics and Strength of materials (Elastostatics) such as its location determines in the crossing of these sciences.

The quality and operational indicators of the machines and equipment considerably depend on the mechanical and physical properties of materials of their constructional elements. Traditional methods of the strength of materials for the determination of mechanical parameters of constructional elements aren't reliable and accurate today. Therefore, there is a need to investigate and specify mechanical characteristics of materials at the level of nanoparticles. For the representation of real values of mechanical characteristics of materials, it is necessary to investigate their nanostructures and crystal lattices. Theoretical and experimental researches of mechanical characteristics of materials without any hypothesis and assumptions are including to the Nanomechanics subject. Here the hypotheses of continuity of material are absent and the research of anisotropic characteristics of the material is conducted taking into account discrete properties of their internal structures. And it causes to increase the quality indicators of machines and mechanisms.

In recent years the numerous works are published on the problems of Nanomechanics in this area. In the field of dynamic analyses of crystal lattices of metal structures works [1-3] the classical available. In the following works, the methods of definition of elastic characteristics of monocrystals on the basis of M. Born theory [1] are developed.

Recently there were many works in the field of research of mechanical characteristics of the nano measured objects, such as in works [4, 5] the mechanical model describing a two-dimensional hexagonal crystal lattice is presented. It is shown that a pair of moments of interaction can provide the stability of such lattice. The generalized moment potential describing the interaction of particles in general view is allowing to set the relations of stiffness, consistent with experimental data. The features of bending stiffness of nanocrystals and nanodimensional structures are investigated and defined the moment of the interaction of nanostructures [6, 7]. In the works [8-11] the features of bending stiffness of nanostructures of materials are considered and the characteristics of interactions of these parameters are defined. There are investigated the van der Waals forces, the Lennard-Jones and Morse potentials and other parameters having important practical value for determination of actual mechanical parameters of materials in some works [12-14].

The principles and conceptions of mechanics of a deformable solid body are considered in [15-17] which are the basis for studying the mechanical characteristics of materials.

The goal of the work to study the mechanical properties of the machine parts are used in oil and gas industry is based on the principles of Nanomechanics. The results of the research is the using it use in oil and gas pipelines which can use in the design and operation.

In view of the discussion and, in particular, the criticism concerning the Nanomechanics theory of potential force field in the nanostructure is thought that it may be of some interest to present, in that follows, a reformulation of the general theory given in [1-3] with the following aims:

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- accounting for the criticism concerning the mechanical motion of the nanodimensional particle approximation of the following the ideas presented in the result of this investigation;
- justification of neglecting the external forces in the differential equations of the mechanical motion, while retaining it in the nanoparticles of the surface, as proposed in micro- and quantum mechanics [18];
- obtaining explicit expressions (rather than the implicit relations are given in classical strength of materials) for the determination the mechanical properties of materials in order to make the theory immediately applicable to particular problems. This may also foster various applications, e.g., the modulus of elasticity ones.

II. Describing the potential force field of the nanostructure and its potential function

The monocrystal structure of the material can be shown as a force field of the crystal lattice, where on its knots are placed the nanoparticles. In other words, we considered a discrete internal structure of the material which is filling with force fields. It characterizes the real situation of anisotropic properties of the material [19, 20].

It should be noted that nanostructures of material are characterized by parameters of their lattices, i.e. by distances between particles on an edge of an elementary cell. Parameters of cubic lattices are characterized by a length of an edge of a cube and denoted by a letter *a*. The hexagonal lattice is characterized by two parameters - the length of hexagon *a* and prism height *h*. When the parameter of the crystal lattice is *k=h/a = 1,633*, the atoms are packed most densely, and the lattice is called the compact hexagonal. Some metals have a hexagonal lattice with less dense packing of atoms (*k >1,633*). The lengths *a* of cubic lattices of metals are ranging from 0,286 up to 0,607 nanometers. The parameter *a* is ranging in 0,357 - 0,652 nanometers and the parameter *h* lies within 0,228-0,398 nanometers for metals with a hexagonal lattice [21-23]. According to Microcontinuum Field Theory [24] of the force field at any point in an elastic continuum does not only depend on the strain field at the point (hyperelastic case) but also on strain at all other points of the body. A. Eringen [24, 25] attributed this fact to the atomic theory of lattice dynamics and experimental observations on phonon dispersion.

Let us consider a particle of nanostructures moving in the potential force field under acting the force which depends on the coordinates of its point of application *x, y* and *z*. Then the projections of the force *F* of the field have been presented by the following expressions [2]:

$$F_x = F_1(x, y, z), F_y = F_2(x, y, z), F_z = F_3(x, y, z). \quad (1)$$

The elementary work done by the force *F* is equal to the differential of potential function $U(x,y,z)$ of a force field in negative sign.

$$dA = F_x dx + F_y dy + F_z dz = -dU(x, y, z). \quad (2)$$

Integrating the equation (2) we will get a full work of potential force *F:*

$$A_{01} = -\int_{M_0}^{M_1} dU(x, y, z) = U_0 - U_1, \quad (3)$$

where $U_0(x_0, y_0, z_0)$ and $U_1(x_1, y_1, z_1)$ are values of the potential function in initial and final points of motion M_0 and M_1 respectively.

So, the work of the potential field force is equal to the difference of values of potential functions in final and starting points of its way and does not depend on the type of a trajectory of a moving particle. Therefore, when the motion occurs in the closed trajectory here is $U_1(x_1, y_1, z_1) = U_0(x_0, y_0, z_0)$ and the work of the potential field force is equal to zero. The main property of a potential force field is that the work of the field force depends only on initial and final positions of the moving particle and neither depends on a type of its trajectory, nor on the law of the motion.

From the above mentioned follows that using the potential function, it is possible to determine the force acting on any point of the field. From Eq. (2) by calculating the differential of function $U(x, y, z)$ we determine the projections of force acting in the potential force field [2, 18]:

$$F_x = -\frac{\partial U}{\partial x}, F_y = -\frac{\partial U}{\partial y}, F_z = -\frac{\partial U}{\partial z}. \quad (4)$$

Thus, the projections of force on the coordinate axes in a potential force field are equal to the private derivatives of the potential function with respect to the corresponding coordinates, i.e. $\bar{F} = -grad\, U(x, y, z)$. From expressions (4) we find:

$$\frac{\partial F_x}{\partial y} = -\frac{\partial^2 U}{\partial x \partial y}, \frac{\partial F_y}{\partial x} = -\frac{\partial^2 U}{\partial x \partial y} \text{ and so on.}$$

From here follows that if the force field is a potential field, the private derivatives of the projections of force are equal each - other:

$$\frac{\partial F_x}{\partial y} = \frac{\partial F_y}{\partial x}, \frac{\partial F_y}{\partial z} = \frac{\partial F_z}{\partial y}, \frac{\partial F_z}{\partial x} = \frac{\partial F_x}{\partial z}. \quad (5)$$

The conditions (5) are necessary and sufficient conditions of the fact that the force field is potential. Thus, if the force of the force field is determined by the equations (1), then using the conditions (5) is possible to establish that this field is potential or not. If the field is potential, then with using the Eq. (4)

and (3) can be determined the force and the work of the force of the potential field.

Generally, in practice are using a 2-d grade Lagrangian Eq. for describing the mechanical motion of a system of interacting material particles having n degrees of freedom [2, 18, 19].

III. Describing the motion of a nanoparticle and the mechanical properties of the material

In the Fig. 1 is shown crystal lattices in knots which are elementary particles the sizes less than 100 nanometers in 3-dimensional format (the third size is accepted as unit one). Here internal crystal lattices are presented as the mechanical system of material particles moving in the force field. It should be noted that in macro mechanics the sum of internal forces is accepted equal to zero. But, as it is noted above, at the interaction of nanodimensional particles internal forces content change his classical contents and are determined by potential functions of a force field. There are external forces acting on nanoparticles of crystal lattices aren't considered here. Therefore, the deformation condition of a monocrystal depends on distances a - between nanoparticles and the distances h - between crystal layers. Force of the interaction of two nanoparticles is defined as force $F(r)$ of the potential force field. As shown in the Fig. 1 each particle is interconnected with other next neighbors particles.

We will consider the motion of any particle M_i in the coordinate system $Oxyz$. On the basis of 2-d grade Lagrangian Eq. can develop the method of described motion of nanoparticles. Analogically and parallel of this method in our case using well-known differential equations of the motion of any nanoparticle of the system may be rewritten as in following ordinary form [2, 18, 23]:

$$m_i \frac{d^2 r_i}{dt^2} = F_i^e + F_i^j \,, \tag{6}$$

where m_i – the mass of a nanoparticle, r_i – radius vector of a particle with respect of a point O, F_i^e and F_i^j are external and internal forces acting on the nanoparticle M_i.
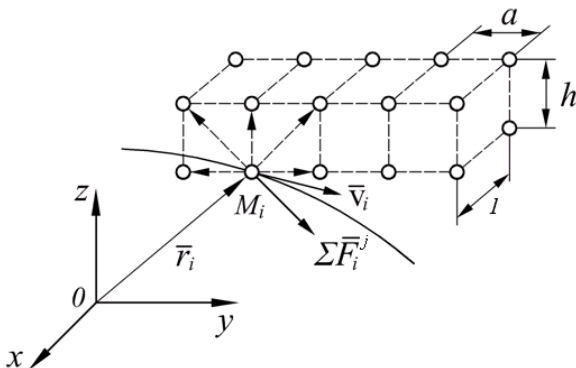

Figure 1. The crystal lattice and movement of nanoparticles in a potential force field.

Note also that in this case the action of external forces on the system aren't considered. On the mentioned theory above the force F_i^j acting on a particle M_i is determined regarding the potential function $U(r_i)$ in the force field.

As mentioned in the Introduction, the most commonly used potential for a force of the field of interactions is the Lennard-Jones potential, which is written in the following form [12-14]:

$$U(r_i) = D \left[\left(\frac{a}{r_i} \right)^{12} - 2 \left(\frac{a}{r_i} \right)^6 \right], \tag{7}$$

where D is the potential energy of constraints, a is the distance between particles in balanced forces of the potential field.

The internal force F_i^j acting on nanoparticles is equal to the force $F(r_i)$ of interaction between particles and is defined from Eq. (4) as the first derivative of the potential function (7) with respect to radius - vector in the opposite sign.

$$F_i^j = F(r_i) = -U'(r_i) = \frac{12D}{a} \left[\left(\frac{a}{r_i} \right)^{13} - \left(\frac{a}{r_i} \right)^7 \right]. \tag{8}$$

Naturally, the vector expression of force acting on the force potential field is

$$\bar{F}(r_i) = F(r_i) \frac{\bar{r_i}}{r_i} = F(r_i) \frac{\bar{r_i}}{a} \frac{a}{r_i} = \frac{12D}{a^2} \left[\left(\frac{a}{r_i} \right)^{14} - \left(\frac{a}{r_i} \right)^8 \right] \bar{r_i}$$

If we are convinced that the field is potential with taking into account Eq. (5), on the basis of the theory mentioned above the elementary work done by a force acting on the potential force field is

$$dA = \bar{F}(r) d\bar{r_i} = -dU(r_i) = \frac{12D}{a} \left[\left(\frac{a}{r_i} \right)^{13} - \left(\frac{a}{r_i} \right)^7 \right] dr_i.$$

Integrating this expression by using the expression (8) we determine the total work as $A_{01} = U(r_0) - U(r_1)$, where $r_0 = a$ and $r_1 = h$ are internal and external values of radius-vector r_i in coordinate system $Oxyz$.

From Fig. 1 we find unit deformations and normal tensions in the direction of a horizontal axis y:

$$\varepsilon = \frac{\Delta a}{a}, \quad \sigma = \frac{F(r_i)}{h} \,, \tag{9}$$

where Δa is absolute elongation in the horizontal direction, $F(r_i)$ is the force acting on the particle and is determined as

$$F(r_i) = c\Delta a, \tag{10}$$

where c is the stiffness of the material is determined as

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$$c = U''(r_i) = -F'(r_i) = \frac{12D}{a^2}\left[13\left(\frac{a}{r_i}\right)^{14} - 7\left(\frac{a}{r_i}\right)^8\right].$$
(11)

Dividing both sides of the Eq. (10) into the unit volume of a particle $V=ah$ (the third dimension is unit 1), we have $\frac{F(r_i)}{ah} = \frac{c\Delta a}{ah}$. Here taking into account the Eq. (9) we have $\frac{\sigma}{a} = c\frac{\varepsilon}{h}$.

The normal tension is

$$\sigma = \frac{ca}{h}\varepsilon = E\varepsilon,$$
(12)

where E is the modulus of elasticity (Young's modulus) of the material. According to Eq. (12) we find $= \frac{ca}{h} = \frac{c}{k}$, where $k = \frac{h}{a}$ - is the parameter of the crystal lattice of the material.

With taking into account the expression (11) we determine the modulus of elasticity as

$$E = \frac{ca}{h} = -\frac{a}{h}F'(r_i) = \frac{12D}{ah}\left[13\left(\frac{a}{r_i}\right)^{14} - 7\left(\frac{a}{r_i}\right)^8\right] = \frac{12D}{V}\lambda^{-8}[13\lambda^{-6} - 7],$$
(13)

where $\lambda = \frac{r_i}{a}$ is the parameter of displacement of nanoparticle in the force field.

Substituting the Eq. (8) to Eq. (6) and without taking into account the external forces we deduced the differential equation the motion of the nanoparticles:

$$m_i\frac{dv_i}{dt} = \frac{12D}{a}\left[\left(\frac{a}{r_i}\right)^{13} - \left(\frac{a}{r_i}\right)^7\right],$$
(14)

where v_i is the velocity of nanoparticle in the potential force field.

The solution of (14) can be found as follows. From the initial condition of the problem, it is known that when $r_i = 0$, the velocity of a particle $v_i = 0$. Taking into account that $m_i\frac{dv_i}{dt} = m_iv_i\frac{dv_i}{dr_i}$, integrating Eq. (14), we will receive:

$$\frac{v_i^2}{2} = \frac{2Da^6}{mr_i^6} - \frac{Da^{12}}{mr_i^{12}}.$$ From here we determine:

$$D = \frac{m_iv^2}{2}\frac{1}{2\lambda^6-1}\lambda^{12} = \frac{K}{2\lambda^6-1}\lambda^{12},$$
(15)

where $K = \frac{mv_i^2}{2}$ is the kinetic energy of the particle.

Substituting the expression (15) to the Eq. (13), we have:
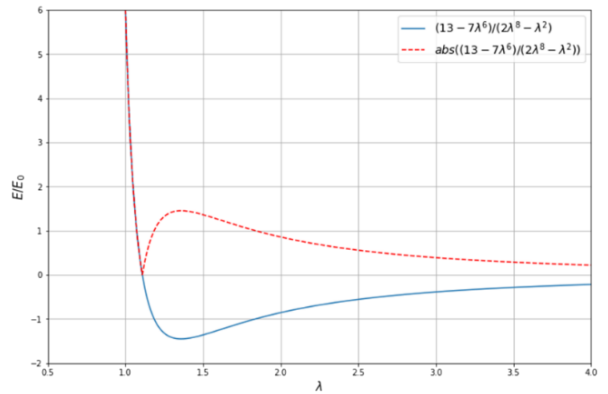
$$E = \frac{12K}{V}\frac{13-7\lambda^6}{2\lambda^8-\lambda^2}.$$
(16)

From here we determine the unit modulus of elasticity (ratio of elasticity modulus) of the material:

$$E/E_0 = \frac{13-7\lambda^6}{2\lambda^8-\lambda^2},$$
(17)

where $E_0 = \frac{12K}{V}$ is the initial dynamical modulus of elasticity of the material.

Using the program Python, we analyzed Eq. (17)

and have been constructed the diagram of the ratio of elasticity modulus E/E_0 with respect to displacement parameter $\lambda=r/a$ of nanoparticle in Fig. 2.

Figure 2. Diagram of the ratio of elasticity modulus with respect to displacement parameter λ=r/a

The analyses of the nanostructures of materials are showed that the elastic characteristics of the material in macro and micro levels significantly different in each other. Furthermore, it follows from (17) with (15) that the ratio of the modulus of elasticity depends on displacements of nanoparticles in a potential force field.

IV.   Formulation of the results of the researches

In this paper, the method of the definition of the mechanical properties of materials in nano-dimensional levels is developed. The essence of the method is that on the basis of the diagram (Fig. 2) and expression (16) with taking into account the expression (13) is determined the ratio of elasticity modulus E/E_0. Then for each given k=h/a values of the parameter of the crystal lattice can be determined the values of elastic characteristics of the given materials (modulus of elasticity, the coefficient of stiffness, etc.). Thus, neglecting the external forces, the analytical method is established to specify the mechanical properties of the materials at the level of nanoparticles.

V.   Conclusions

The mathematical modeling of the mechanical properties is considered and the internal structure of the material is investigated on the basis of principles of Nanomechanics with taking into account of the nanoporous gaps between nanoparticles. Here the isotropy and continuity characteristics of materials are neglected, deduced and solved the differential equations of motion of nanoparticles in potential force field on the basis of Lennard-Jones potential

function. Here is established that the modulus of elasticity of materials is changing depending on distances between gaps of particles belonging to the crystal lattice. In result, we determined the potential field force, the work done by the field force and deduced the practical expressions and diagrams for determination of real elasticity properties of materials.

The results of researches can be useful for increasing the accuracy and reliability of machine parts during the calculating and choosing of their materials.

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