Probabilistic Approach to Damage Modeling of Aviation Composite Materials

Vyacheslav Astanin, Oleksii Olefir, Ganna Shchegel, Andrii Olefir
National Aviation University
1, Kosmonavta Komarova ave., Kyiv, 03058 Ukraine

Abstract

Probabilistic model of damage calculation for aviation composite materials is proposed, the main task of which is physically substantiated modeling of stress dependence on deformations under the influence of external loading, distinguishing between the formed elastic and plastic deformation, as well as irreversible cracking and material destruction. For this purpose, the calculation of the probabilities of the destruction of bonds between the material elements, as well as the equivalent energy of deformation is made. Comparison of the results of numerical calculations with experimental data shows principal applicability of the proposed model.

1. Introduction

Modeling the behavior of multicomponent composite materials made on the basis of particles or fibers as a reinforcing phase, as well as various types of plastic or metal matrices as a binding phase, and which are widely used in modern aviation, in spite of all their diversity, is associated with the same typical problems as the simulation of traditional structural metals and alloys. In particular, in order to describe the behavior of materials of both types, specialized models are widely used, which are well adapted for certain temperature ranges, loads or other conditions of interaction, but are difficultly generalized to wider ranges of operating conditions [1-3].

At the same time, when choosing a particular calculation model, it is often necessary to operate with a set of material properties, which are often more qualitative than quantitative [4, 5]. Such properties determine the choice of a model, but are not explained by the model itself. For example, these characteristics are material brittle or plastic behavior, relationship between static and long-term durability, creep and strengthening, yielding and melting heat.

On the other hand, it is known that only a few typical atomic gratings and types of molecular bonds exist, which result in ionic, covalent, van der Waals bonding, also an additional effect of molecular bonds due to vulcanization can be considered. Moreover metals for example can be also potentially unified as the calorimetric properties of metals in general are similar if some magnitude factor is introduced which depends on the atomic structure and Debye temperature [6].

Thus, the question arises as how it is possible to describe the mechanical behavior of a material, based not so much on the phenomenological data about each particular material [7, 8], but from the general physical analysis grounded on its basic parameters, such as atomic mass, interatomic distance, coefficients of the function of potential energy of interatomic interaction and other similar quantities [9, 10].

The immediate task that needs to be solved to answer the question is to establish a quantitative relationship between the loading conditions, conditions of the experiment and the mechanical behavior of the material. In this study, the solution of this problem is presented for the case of stress and strain simulation of simple composite elements based on a metal matrix, using a probabilistic approach.

2. Materials and methods

The study was implemented in three stages, with the transition from analysis of a simple material without strengthening, which is characterized with an expressed ductile behavior, then of a non-reinforced material, which is characterized with more brittle behavior under the given conditions of the experiment conducting, to the analysis of the latter in the role of a matrix of reinforced with particles metal composite.

Thus, at the first stage of the simulation, an attempt was made to predict the uniform tensile loading of a standard cylindrical specimen made of almost pure metal without the use of reinforcing particles. As such a material, a solid low-carbon solution in iron, namely ferrite, was considered, since the properties of the ferrite are rather close to the

Vyacheslav Astanin, Oleksii Olefir, Ganna Shchegel, Andrii Olefir

properties of pure iron, and therefore carbon inclusions can be neglected when modeling the phonon effects of the impact on the strength of the material. The mechanical characteristics of the material are given in Table. 1 [11].

Table 1: Mechanical characteristics of ductile ferrite specimen

	Proportionality limit	Plasticity limit	Ultimate strength	Young's modulus, $_1$ GPa
Stress, MPa	184,45	275,60	345	1,085
Strain, %	0,17	0,37	25	1,085

In order to test a comparatively more brittle material, a specimen made of cast aluminum alloy was selected, the mechanical characteristics of which are given in Table 2 [11, 12].

Table 2. Mechanical characteristics of brittle aluminum specimen

	Proportionality limit	Plasticity limit	Ultimate strength	Young's modulus, 10^2 GPa
Stress, MPa	283	345	414	0,69
Strain, %	0,41	0,52	0,98	0,69

In the third stage of the study a composite material was tested, for which a specimen of a powder composite was used representing a matrix of aluminum alloy A359 reinforced with particles of silicon carbide. The mechanical characteristics of the material are given in Table. 3 [13].

Table 3. Mechanical characteristics composite specimen based on aluminum

	Proportionality limit	Plasticity limit	Ultimate strength	Young's modulus, 10^2 GPa
Stress, MPa	80	130	245	0,67
Strain, %	0,12	0,21	1,25	0,67

3. Probabilistic approach to modeling of materials

Structural elements of a material at different scales, namely the nano-, micro- or macro-scales, are interconnected by force interaction. A hypothesis was put forward that mechanical behavior of a material is determined by the ratio of the time during which this force interaction manifests itself at a level sufficient for providing significant influence on the course of the phenomenon under study, namely, the appearance of internal stresses in the material in response to external force or temperature influences, and this case is terminologically referred to as the existence of a connection or bond between the said structural elements, and the time during which this force interaction manifests itself at a level which is, on the contrary, insufficient for the indicated significant impact, that is terminologically designated as the absence or destruction of the bond.

Below we consider the peculiarities of the formation and the temporal stability of this characteristic, namely the force interaction between the structural particles of the material, in detail, in order to establish, in particular, whether it relates to those parameters whose discreteness of change can be neglected, that is, if the transition from the presence of a bond to its absence and vice versa is intermittent or continuous.

It is known that atomic particles in a solid body are in a state of continuously maintained dynamic equilibrium of thermal vibrations of atoms. The calculation of the distribution of internal energy of a solid body between oscillations of different frequencies and spatial wavelengths can be carried out using the Bose-Einstein or Maxwell-

Boltzmann statistics for the so-called large canonical ensemble of indistinguishable quasiparticles – phonons – each of which corresponds to oscillations of a certain frequency.

With this approach to modeling there is a certain paradox. Usually, the presence of sufficient energy for activation of phonons of a certain frequency and amplitude is interpreted as the presence in the material of some number of atoms with the energy of exactly this magnitude, and the percentage of these atoms corresponds to the probability of particles to occupy the corresponding energy level.

However, in this case there is a theoretical problem, as this approach to modelling cannot explain the presence of time dependence of the material's reaction on the load, which has its manifestation in the phenomena of long-term durability and material strengthening in case of growth of the strain rate, because the properties of the material are treated as being stationary in time.

The solution of this paradox is suggested in this study on the basis that the described treatment of the probability of taking certain energy levels in a material contradicts the principle of ergodicity of the system, which, along with the principle of the indistinguishability of the particles (that is, the principle of a priori probability) and the principle of maximization of entropy, forms the basis of statistical mechanics.

Explanation is as follows. In accordance with this principle, in the case of considering quasiparticles, such as phonons, having a zero chemical potential for adding a new particle to the system, that is, the number of particles in the system is unlimited, in fact not a number of phonons of a certain frequency should be considered, but the number of energy levels of one and the same the only single phonon. Hence the spatial statistical distribution of probabilities of the system energy levels and its equivalence to the mean time values of the corresponding physical quantities cannot take place. That is, on one side, the ergodicity of the system manifests itself in the spatial and temporal relation of energies of different phonons in space and time. But on the other side, when it comes to a certain phonon of a given frequency, realization of different amplitudes of oscillations does not occur simultaneously in different points of the material, but it occurs consistently over time with a certain frequency.

Let's consider the theoretical dependence of the energy of interaction between two structural particles on the distance between them (Fig. 1). Each energy level n of a phonon of a given frequency ω and full energy $E_n = (n + \frac{1}{2}) \cdot \hbar \cdot \omega$, where $\hbar$ – Planck constant, $\frac{1}{2} \cdot \hbar \cdot \omega$ – energy of a zeroth energy level, corresponds an oscillations of a certain amplitude. According to an idealized curve, at a certain distance $x_{\min}$ between particles, a minimum of potential energy $E_n(x_{\min} / x_0)$ of their interaction is observed (Fig. 1, a). However, according to a quantum-mechanical approach, a wave function $|\psi_n|^2$, which describes the state of the microsystem, can take only discrete values. Fig. 1, b schematically shows the number of local minima of the function $|\psi_n|^2$ at each energy level n, which is numerically equal to n and also numerically equal to the conditional number of quasiparticles – phonons, which, as it is terminologically designated, are present at this energy level.

In fig. 1, b the amplitude of oscillations is determined along the horizontal axis and equals to half the width of the plot of the horizontal line corresponding to a certain n, where this plot is limited by the curve of energy dependence on the distance.

On the other hand, when the amplitude of the oscillations exceeds some critical level, so that the particle enters the region $x < x_0$, when $E_n \geq 0$, or the region of such $x >> x_0$, so that $E_n \approx 0$, then the level of the potential energy of interaction of the particles becomes not high enough to prevent getting into the sphere of influence of other neighboring particles. Corresponding additional displacement and associated irreversible deformation take place. Since the energy levels of the phonons are discrete, so the excess of the critical amplitude and energy of the oscillations, which correspond to the occurrence of bond destruction, is abrupt. Accordingly, the presence and absence of the bond between any structural particles of a material are two separate discrete states in the process of evolution of material deformation and damage.

Another important conclusion regarding the peculiarities of the transition between energy levels, which correspond to oscillations of bound particles (described with probability p_r), and energy levels, which correspond to the bond destruction (described with probability p_f, both probabilities p_r and p_f can be calculated according to [14-16] and their graphs are shown in Fig. 1, c), is that at any of them the probability that the amplitude and accordingly the energy of the oscillation reaches some higher value, which even corresponds to higher energy levels, is nonzero. And as it is shown above, such transitions to higher energy levels, in particular those at which the bond turns out to be destructed, occur not continuously with different particles of the material, but consistently, once pro a certain number of oscillation cycles (since the phonon under consideration can be brought into conformity with some certain oscillation frequency), but in the whole volume of the material, as in fact only one single quasiparticle, phonon, is present in the entire material volume, and this unitary quasiparticle describes the oscillations of the considered frequency.

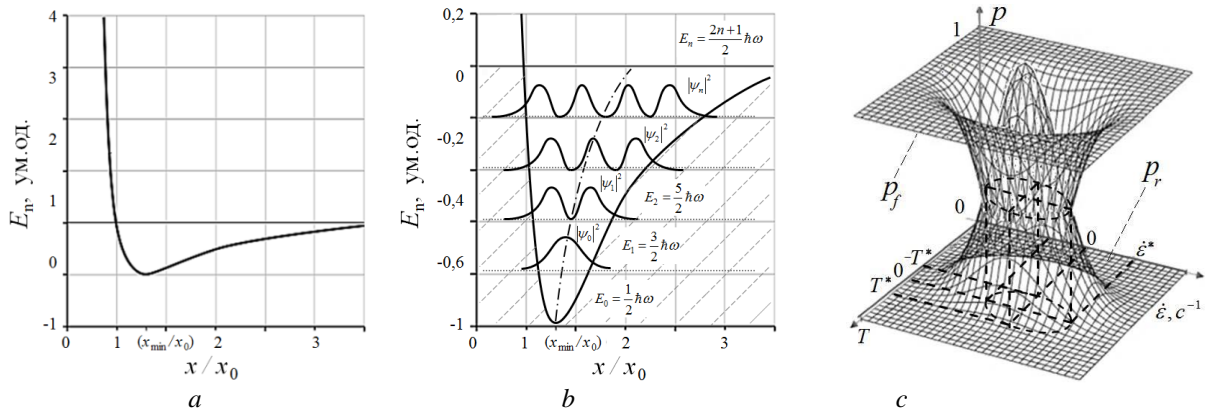Vyacheslav Astanin, Oleksii Olefir, Ganna Shchegel, Andrii Olefir

Figure 1: Dependence of the energy E_n of interaction between the two structural particles on the relative distance x_0/x between them: a – theoretical curve; b – illustration of the quantum-mechanical approach; c – graphs of functions $p_f(\dot{\varepsilon},T)$ and $p_r(\dot{\varepsilon},T)$

An additional confirmation of relevancy of the suggested interpretation is the very definition of a phonon quasiparticle as of a joint oscillation of the entire n-dimensional chain of interacting physical particles. It exists only if all of them together participate in this oscillation.

It is also worth to note the appropriateness of distinguishing between two main types of bonds between any material structural particles, namely the normal and the tangential or the shear bonds, which correspond to the known from mechanics of materials and structures main types of stresses with the same names, as it was proposed and discussed in detail in [9, 10]. In this case, rupture of the former ones, namely of the normal bonds, corresponds to the possibility of fracture of the material specimen into parts, rupture of the latter ones gives the opportunity of forming plastic deformations due to the slip of material layers, which has its manifestation in the form of motion of dislocations.

Obtained solution of the problem with the help of the described probabilistic approach allows determination of the following stages of further modeling of the material mechanical behavior: calculation of the probability of energy levels occupation of the phonons of a selected frequency; determination of critical amplitudes corresponding to destruction of bonds between atoms; calculation of probabilities of exceeding these critical amplitudes; calculation of the frequency of exceeding the critical amplitudes of oscillations; calculation of the probabilities of destruction of normal and tangential bonds; calculation of probabilities and frequencies of critical combinations of destruction of normal and tangential bonds that lead to certain types of damage (here, by the way, one can refer to the widely used concept of phenomenological differentiation of various types of damage in composites [17-20] – warping, cracking , fiber pull-out etc., for which the application of the proposed probabilistic approach allows, therefore, to provide a quantitative assessment during modeling and simulation, as well as, as it will be seen from the results below, to predict which type of damage prevails and hinders development of the others); calculation of equivalent strain rates corresponding to each type of damage; a stepwise calculation of the material reaction to loading with simultaneous determination of the fractions of ductile, or plastic, and so-called diffuse deformation (damage) and equivalent energies, namely the potential energy of elastic deformation, plastic deformation, heat losses; calculation of the corresponding stresses; determination of the critical points of irreversible destruction when the probability p_f of bond destruction excesses the probability p_r of its integrity or restoration.

4. Methodology of numerical modeling

The number N_λ of permitted wavelengths λ_i in a material specimen, and hence the number N_ω of permitted phonon frequencies ω_i, is equal to the number of atoms N_x in the chain of material particles along a given specimen dimension, for example, along the x axis, i.e.

$$N_\omega = N_x,$$ (1)

where numbering starts from $-\dfrac{N_x}{2}$ then through 0 to $+\dfrac{N_x}{2}$.

The internal energy of material specimen U is distributed between phonons of different frequencies with equal probability. At a given moment of time, a phonon of some specific frequency may obtain all the internal energy U of the material specimen, or some certain part of the energy or no part of it, that is, a phonon does not manifest itself, in other words oscillation of the corresponding frequency does not manifest itself. Moreover, if the part of U, which is related to a considered phonon at a given moment of time, is less than necessary for existence of at least one phonon from the point of view of energy quantization properties, then it does not manifest itself, that is, its amplitude is zero. Depending on the magnitude of the part of the energy U, which is related to the phonon of the considered frequency at the given moment of time, this phonon may appear, as already mentioned, with zero amplitude, single, double amplitude, etc., that is terminologically denoted as the presence of correspondingly zero, one, two or more of the phonons of this frequency.

Consequently, if the number of allowed phonon frequencies is N_ω, then at a certain moment of time the internal energy U of the material specimen can be distributed to only one of them in a unique way. But since their number is N_ω, so the total amount of ways for distributing the energy U to only one phonon of N_ω phonons is equal to

$$C_{N_\omega}^1 = \frac{N_\omega!}{(N_\omega - 1)! \cdot 1!} = N_\omega. \tag{2}$$

For an arbitrary number m of phonons to which the energy U is distributed, where $1 \leq m \leq N_\omega$, the formula for the number of ways gives the number of methods of how to choose m from N_ω according to the rule of combinatorics for the number of combinations:

$$C_{N_\omega}^m = \frac{N_\omega!}{(N_\omega - m)! \cdot m!}, \quad 1 \leq m \leq N_\omega, \ m \in Z. \tag{3}$$

Thus, the total number of ways or methods for distributing the energy U among one, several or all phonon frequencies:

$$C_{N_\omega}^{1\,\text{II}\,2\,\text{II}\,\ldots\,\text{II}\,N_\omega} = \sum_{m=1}^{N_\omega} C_{N_\omega}^m = C_{N_\omega}^1 + C_{N_\omega}^2 + \ldots + C_{N_\omega}^m + \ldots + C_{N_\omega}^{N_\omega - 1} + C_{N_\omega}^{N_\omega} =$$

$$= \frac{N_\omega!}{(N_\omega - 1)! \cdot 1!} + \frac{N_\omega!}{(N_\omega - 2)! \cdot 2!} + \ldots + \frac{N_\omega!}{(N_\omega - m)! \cdot m!} + \ldots + \frac{N_\omega!}{(N_\omega - (N_\omega - 1))! \cdot (N_\omega - 1)!} +$$

$$+ \frac{N_\omega!}{(N_\omega - N_\omega)! \cdot N_\omega!} = N_\omega + \frac{N_\omega!}{(N_\omega - 2)! \cdot 2!} + \ldots + \frac{N_\omega!}{(N_\omega - m)! \cdot m!} + \ldots + N_\omega + 1 \tag{4}$$

or

$$C_{N_\omega}^{1\,\text{II}\,2\,\text{II}\,\ldots\,\text{II}\,N_\omega} = \sum_{m=1}^{N_\omega} C_{N_\omega}^m = \sum_{m=1}^{N_\omega} \frac{N_\omega!}{(N_\omega - m)! \cdot m!}, \tag{5}$$

where

$$C_{N_\omega}^1 = N_\omega, \quad C_{N_\omega}^{N_\omega - 1} = N_\omega, \quad C_{N_\omega}^{N_\omega} = 1. \tag{6}$$

Vyacheslav Astanin, Oleksii Olefir, Ganna Shchegel, Andrii Olefir

So there is a need to calculate a large number of factorials of numbers much larger than 10^2, which causes numerical difficulties (memory overflow when storing floating-point numbers). Therefore, in order to calculate factorials, the following mathematical approach is used. The function Γ is introduced so that $\Gamma(n+1) = n!$, and an approximate Stirling formula is utilized [21]:

$$\log \Gamma(x) \approx (x - 1/2) \log(x) - x + (1/2) \log(2\,\pi) + 1/(12\,x) - 1/(360\,x3) + 1/(1260\,x5) - \dots \tag{7}$$

Additionally, in order to simplify the calculation of the sum of combinations $C_{N_\omega}^m$, where $1 \le m \le N_\omega$, $m \in Z$, from a mathematical point of view, it was noticed that for large numbers N_ω the values of $C_{N_\omega}^m$ are distributed close to the normal law: graph of the function $f_C(m) = C_{N_\omega}^m(m)$ practically coincides with the scaled graph of the

Gaussian function $f_G(m) = \dfrac{1}{\sigma \cdot \sqrt{2\pi}} \cdot e^{-\frac{(m-\mu)^2}{2 \cdot \sigma^2}}$, where $\sigma \in R, \mu \in R$, that is, they are similar to each other.

Since the Gaussian function describes the normal probability distribution for a one-dimensional case, we can use the terms for the parameter μ – mathematical expectation (mean), median and mode of the distribution, and for the parameter σ – mean square deviation, for σ^2 – dispersion of the distribution.

Then the normal distribution of probabilities for the one-dimensional case acquires the following physical meaning: for a large number of possible and equally probable ways of how to distribute the internal energy of a material specimen between phonons of different frequencies and amplitudes, the density $f_G(m)$ of probability to involve a certain number m of phonons of different frequencies is equal to the number of combinations $C_{N_\omega}^m$, with the help of which exactly this number m of phonons of different frequencies can be chosen among all allowed phonons N_ω.

Therefore the most expected situation is the one when the number $\mu = \dfrac{N_\omega}{2}$ of phonons is involved, because the number combinations in this case reaches the maximum. It was shown that dispersion of such the distribution is $\sigma^2 = \dfrac{N_\omega}{4}$, mean square deviation is $\sigma = \dfrac{1}{2} \cdot N_\omega^{\frac{1}{2}}$, or, using adjusted calculations for the case $N_\omega \le 100$, mean square deviation is $\sigma = 0{,}515 \cdot N_\omega^{0{,}495}$.

For a multidimensional case of the normal probability distribution, it is considered expedient to explain its physical meaning in the similar way to the one-dimensional case, but considering phonon oscillations or vibrations of not one-dimensional, but two-, three- or multidimensional chain of particles of the material.

It is worth noting that it is possible to perform interpolation of the graph of the function $f_C(m)$ for a non-discrete m in view of the fact that due to the property of quantization of the phonon energies only an integer number of phonons can physically appear, i.e. be registered – even if some amount of energy is allocated at the current moment of time for the phonon of a given frequency, such that this amount is greater or possibly smaller than the amount corresponding to their nearest integer number. This means that non-integer combinations of variants are still theoretically possible and must play their important role in the calculations, although the mathematical apparatus for non-integer combinations is not trivial.

Moreover, if we analyze this phenomenon in more detail, it turns out that the point is not even in a mandatory implementation of the phonon amplitude, which corresponds to the internal energy allocated to it at the current time moment, but only in the probability of realizing a phonon of one or another quantized amplitude at the given level of the average energy.

Thus, interpolation and extrapolation of the graph of the function $f_C(m)$ for non-discrete quantities of phonons $m \in R$ means either (1) – the presence of energy fluctuations, which are not sufficient for the transition of a phonon to the next energy level, that is, to the next quantized amplitude value, but which are present during fractions of a second for the allowed phonon frequencies, whether they are allowed is determined by the interatomic distance of the particles and their number in the chain, and thus it means that there are deviations from the ideal distribution in the real physical body, or (2) – the realization of these frequencies of phonons, which are not allowed in the case of the ideal model of a solid body, and these phonon frequencies correspond again to either integer quantized amplitudes or these amplitudes and additional energy fluctuations.

Conclusions are as follows. In the case of interpolation and extrapolation of the function graph $f_C(m)$ for non-discrete quantities of phonons $m \in R$ we obtain an area under the function graph $f_C(m) = C_{N_\omega}^m(m)$, which is numerically equal to the sum of such quantities, each of which is equal to the number of variants of how to distribute the internal energy of a material specimen between a certain number of phonons of different frequencies. Arbitrary, not obligatory integer or finite numbers of phonons and frequencies are considered. And additionally it turns out that, in fact, the portion of those variants, which are related to the physically nonrealistic phonon frequencies according to the classical theory of solid body, is very small compared to the energy levels permitted by this theory. Moreover, as it will be seen below, the specific portion of energy expended on these unrealized frequencies varies depending on the number and the frequency range that are allowed in this particular material specimen, given its geometric dimensions and the type and distance between oscillating particles.

Thus, the described area under the curve $f_C(m)$, which is equal to the sum of the variants of the distribution of the internal energy of the material specimen among all possible phonons of different frequencies and amplitudes, can be approximated to be an area under the graph of the Gaussian function $f_G(m)$, since these two graphs are similar:

$$\frac{Area(f_G(m))}{Area(f_C(m))} = \frac{f_G(\mu)}{f_C(\mu)} \tag{8}$$

or

$$\frac{\int\limits_{-\infty}^{+\infty} f_G(m)dm}{\int\limits_{-\infty}^{+\infty} f_C(m)dm} = \frac{f_G(\mu)}{f_C(\mu)}. \tag{9}$$

As it can be seen from the equations above, the similarity coefficients between the normalized to the unit area $\int\limits_{-\infty}^{+\infty} f_G(m)dm = 1$ under the graph of the normal probability distribution function $f_G(m)$ and the area under the graph of the function of the sum of the variants of energy distribution between the phonons of the specimen $f_C(m)$ is equal to the ratio of the values of these functions at abscissa, which is equal to the mathematical expectation $\mu = N_\omega / 2$, which can easily be calculated directly for $f_G(m)$ and if to apply the above-mentioned Stirling formula also for $f_C(m)$.

We further consider that each individual variant of the distribution of the body internal energy between phonons is a separate microstate within the macrosystem of the material specimen. We introduce for the total number of microstates of the system the traditional designation Ω [22]. Then for exclusively integer discrete states of the macrosystem:

$$\Omega = \sum_{m=1}^{N_\omega} C_{N_\omega}^m, \tag{10}$$

and in the case of taking into account possible energy fluctuations and the influence of additional oscillation frequencies:

$$\Omega = \int\limits_{-\infty}^{+\infty} f_C(m)dm = \frac{f_C(\mu)}{f_G(\mu)}, \quad \mu = N_\omega / 2. \tag{11}$$

Vyacheslav Astanin, Oleksii Olefir, Ganna Shchegel, Andrii Olefir

The latter case includes also fluctuations and frequencies due to the occurrence of local phonon modes, which are caused in particular by the non-homogeneity of the structure of the three-dimensional chain of particles within the material specimen, such as lattice defects, vacancies, dislocations, faces of grains, etc., or by impurities and inclusions.

It should be noted that in the case of applying the expression for the dispersion of the distribution, which as it is shown above is equal to $\sigma^2 = \dfrac{N_\omega}{4}$, the formula for the normal distribution of probabilities can be presented as:

$$f_G(m) = \frac{1}{\pi \cdot k} \cdot e^{-(\frac{m}{k} - k)^2} , \quad \text{where} \quad k^2 = \mu . \tag{12}$$

In particular

$$f_G(\frac{N_\omega}{2}) = \frac{\sqrt{2}}{\pi \cdot \sqrt{N_\omega}} . \tag{13}$$

With the calculated number Ω of microstates of the system, the conclusion is derived that indeed the probability of occurrence of each individual phonon according to the very definition of the mathematical notion of probability cannot exceed unity, but the number of ways in which these phonons may emerge, that is, the ways in which the available internal energy of the material specimen can be allocated to them, is allowed to exceed and usually exceeds unity.

The following considerations demand now a deeper analysis of the physical meaning of the number of microstates Ω of the system. We assume, as before, that every microstate is equally probable, and hence, the probability of occurrence of each of these microstates:

$$p_\Omega = \frac{1}{\Omega} . \tag{14}$$

Every microstate is a case in which all internal energy of the body is spent on the occurrence of elastic oscillations at frequencies of a certain range and discreteness, that is, of a certain sample of frequencies, with all frequencies equally probable, but the samples are also equally probable, and therefore, the presence of any frequency in the sample is also equally probable.

At any given moment of time the energy can be spent on the occurrence of only one oscillation of some frequency, that is of only one single phonon and the sample contains only one frequency, or on combined oscillation of some two frequencies, i.e. the sample contains two arbitrary frequencies from the allowed range, that corresponds to two phonons, etc. up to the realization of all the permitted frequencies at once, i.e. N_ω phonons at once. To avoid terminological uncertainty, we avoid the notation of a phonon of n-th amplitude as of a multitude of n phonons, which is often used in the literature [22, 23]. That is, we use the notation according to which we speak of the presence of only one phonon of a certain frequency, which is realized with the amplitude of n-th order, since the amplitude is quantized, as opposed to saying that there are n phonons implemented at this frequency. Thus if only one phonon is realized at a given time moment, that is, all the energy is spent to its manifestation, then the amplitude of this phonon is higher in comparison with the case when the same total internal energy is distributed among a greater number of phonons. Then the probability of occurrence of a separate phonon, if it is the only phonon manifested at the given time moment, is equal to $p_1 = p_\Omega = \dfrac{1}{\Omega}$.

If the energy is spent to manifestation of only two phonons at the given time moment, then the probability of any certain two of them $p_2 = p_\Omega = \dfrac{1}{\Omega}$. If it is spent for another certain two phonons, i.e. phonons of arbitrary two other frequencies from the list of allowed ones, then the probability of their manifestation is still $p_2 = p_\Omega = \dfrac{1}{\Omega}$.

The number of variants for choosing two frequencies among N_ω frequencies, as shown above, is equal to $C_{N_\omega}^2$. Thus the sum of the probabilities to choose two random phonons among N_ω phonons is equal to $C_{N_\omega}^2 \cdot p_2$. A general case gives the sum of the probabilities to choose m random phonons among N_ω phonons, where $1 \le m \le N_\omega$, is equal to $C_{N_\omega}^m \cdot p_m = C_{N_\omega}^m \cdot p_\Omega$.

The sum of the probabilities to choose either one or two, or more phonons up to the total number of N_ω phonons, is equal to:

$$P_\Sigma = \sum_{m=1}^{N_\omega} (p_\Omega \cdot C_{N_\omega}^m) = p_\Omega \cdot \sum_{m=1}^{N_\omega} C_{N_\omega}^m = p_\Omega \cdot \Omega = \frac{1}{\Omega} \cdot \Omega = 1 , \tag{15}$$

However, when switching from integer variants of combinations to the environs of the integer values of the number of phonons in the sample, we obtain:

$$dP_\Sigma = \int_{m-dm/2}^{m+dm/2} p_\Omega \cdot dC_{N_\omega}^m = \int_{\theta-d\Omega/2}^{\theta+d\Omega/2} p_\Omega \cdot d\Omega, \quad \text{where} \quad 1 \le m \le N_\omega, \quad 1 \le \theta \le \Omega. \tag{16}$$

Then the sum of probabilities to realize all the possible microstates, which are integer and non-integer microstates in case of fluctuations:

$$P_\Sigma = \int_1^\Omega p_\Omega \cdot d\Omega = \int_1^\Omega \frac{1}{\Omega} \cdot d\Omega = \ln \Omega . \tag{17}$$

Then the value of the average energy of a phonon u_{av}, J, is taken. It is equal to the sum of the average potential and equal to its average kinetic energy of the phonon. And the latter one, in turn, in accordance with the equivalence theorem for thermal equilibrium, is proportional to the body temperature with the Boltzmann coefficient k_B, i.e. $u_{av} = 2 \cdot \dfrac{k_B \cdot T}{2} = k_B \cdot T$. The average energy of a phonon u_{av} is multiplied by the sum P_Σ of the probabilities of occurrence of all the allowed microstates Ω of the system with possible fluctuations (and hence with non-integer intervals), that is, by the sum of the probabilities of variants of how many phonons and which phonons are manifested in the specimen. Then the total internal energy of the material specimen is obtained, as exactly this total internal energy U of the material specimen ensures the manifestation of all the considered microstates:

$$U = u_{av} \cdot P_\Sigma = k_B \cdot T \cdot \ln \Omega = (k_B \cdot \ln \Omega) \cdot T = S \cdot T , \tag{18}$$

where $S = k_B \cdot \ln \Omega$ – the entropy of the specimen in accordance with the definition of entropy in statistical mechanics [24].

In this case, the subject of consideration is not the change in internal energy dU, which could be related to the change in entropy dS when the system is under reconfiguration (melting, boiling), as such a reconfiguration involves the change in the type of permitted fluctuations of the material particles, their frequencies or types of phonons, and hence the change in the number of their possible combinations, thus, the number of microstates of the system, or when the system's volume or the number of material particles in it are changed during chemical transformations.

Contrary to the change in internal energy dU, the whole part U of the internal energy of the material is considered directly (in the context of the questions considered it is the total internal energy U of the specimen), which is related

Vyacheslav Astanin, Oleksii Olefir, Ganna Shchegel, Andrii Olefir

to the mechanical vibrations of its constituent particles, which can be atoms, molecules, grains, etc., that is, to the phonon oscillations.

Based on the considered methodology of entropy and internal energy calculation, the thermodynamic parameters of any given specimen can be determined and then used for calculation of probabilities of destruction p_f or preserving p_r the bonds between material structural elements, while these bonds provide the material strength and resistance to external loading. The following considerations need introducing two equivalent strain rates of so-called diffuse $\dot{\varepsilon}_{eq}^d$ and plastic $\dot{\varepsilon}_{eq}^p$ deformations as it is described in [14-16].

The former equivalent strain rate $\dot{\varepsilon}_{eq}^d$ of diffuse deformation relates to the occurrence of mutually uncoordinated ruptures of normal and tangential bonds between material particles. Displacements of atoms between stationary positions in the lattice occur in this case, but, similarly to what happens in case of other diffuse processes, they occur locally, without being accompanied by organized displacements of the entire atomic planes. Externally, when observed, the described processes are manifested in the form of the motion of dislocations, although their physical basis lies in the destructions and potential renewals of interatomic or intermolecular bonds due to energy fluctuations, which take place in the material and are random but subject to statistical distribution.

The latter equivalent strain rate $\dot{\varepsilon}_{eq}^p$ of plastic deformation relates to the occurrence of phonon fluctuations leading to an organized destruction of bonds during oscillations of particles, when all the lattice atoms are entangled into organized joint vibrational process.

The considered above peculiarities of modeling within the framework of the general calculation algorithm described in the previous section allowed carrying out simulation of behavior of material specimens under loading.

5. Results and discussion

The results of simulation of the stress-strain curves under tension for a ferrite specimen are given in Fig. 2, *a*. Comparison of simulation curve 3 to the experimental curve 2 [11] shows, that deviation of simulation results from experimental data does not exceed 6%. Thin solid horizontal and vertical lines denote in the graphs of Fig. 2 the stresses of the proportionality limit and yielding and corresponding strains. The slanting dotted lines mark dependences of proportionality in accordance with Hooke's law for the considered materials.

The simulation results are thus obtained using the proposed probabilistic approach, i.e. on the basis of calculation of probabilities of destruction and restoration of bonds using the ratio of equivalent strain rates, as presented in Fig. 3, *a*. Considering the dependences of the plastic and diffuse equivalent strain rates, i.e., strain rates corresponding to phenomenological deformations, which are typical for respectively yielding and creep (the latter takes place indeed even at quasi static loading), on strain ε (Fig. 3) reveals the following.

In the first stage, the equivalent strain rate of diffuse deformation of the ductile ferrite specimen exceeds the equivalent strain rate of plastic deformation. It corresponds to the fact that under such low loading conditions the atoms can mutually exchange positions, but the structure of their mutual arrangement remains, plastic deformation, or yielding, practically does not take place. As the abscissa value increases, the difference between the equivalent velocities gradually diminishes leading to that plastic deformations begin to appear gradually.

As then the equivalent strain rate of plastic deformation begins to exceed the equivalent strain rate of diffuse deformation, the manifestation of yielding becomes predominant. And we really observe that as only that happens as indicated in the curves in Fig. 3, the specimen reaches the strains, which correspond to start of yielding, that can be seen in curves in Fig. 2.

Proceeding from the proposed probabilistic approach and the formulated hypothesis, the mechanical behavior of the material is determined by the probabilistic phenomena of interaction of energy fluctuations arising complementary to the background oscillatory processes in the structure of the material. Therefore the proximity of the mechanical properties of ferrite and pure iron can be explained by the fact that, since the density of inclusions of carbon atoms is low, so they result in the occurrence of only local phonon modes without a significant effect on the global energy redistribution between the particles in the specimen under study.

A similar result is obtained for a comparatively more brittle aluminum specimen (Fig. 2, *b*, Fig. 3, *b*). In this case, a sharper transition from the directly proportional dependence to plastic deformation is due to the more significant excess of the equivalent strain rate $\dot{\varepsilon}_{eq}^d$ above $\dot{\varepsilon}_{eq}^p$ before and on the contrary after the critical point of intersection of these curves.

The performed calculations made it possible to proceed to the simulation of composites with a metal matrix (Fig. 2, *c*, Fig. 3, *c*). For the composite, the fracture point is slightly exceeded in comparison with the experimental results according to [13], but, as indicated in the experimental work, there is a significant dispersion of experimental data for

strains exactly beyond the yield boundary. According to the probabilistic theoretical model, the reason for such a pronounced scattering is the asymptotic behavior of the parameter, which is equal to the difference of equivalent strain rates, approaching zero value (Fig. 3, c, the range of strains $\varepsilon > 0{,}2\,\%$). This is just the case when concentrators and material inhomogeneity can play a key role. In the investigated range of parameters the deviation of the stress, which is determined under large strains by random factors of the actual structure of experimental specimens, from the theoretical predicted value constitutes up to 13% (Fig. 2, c).
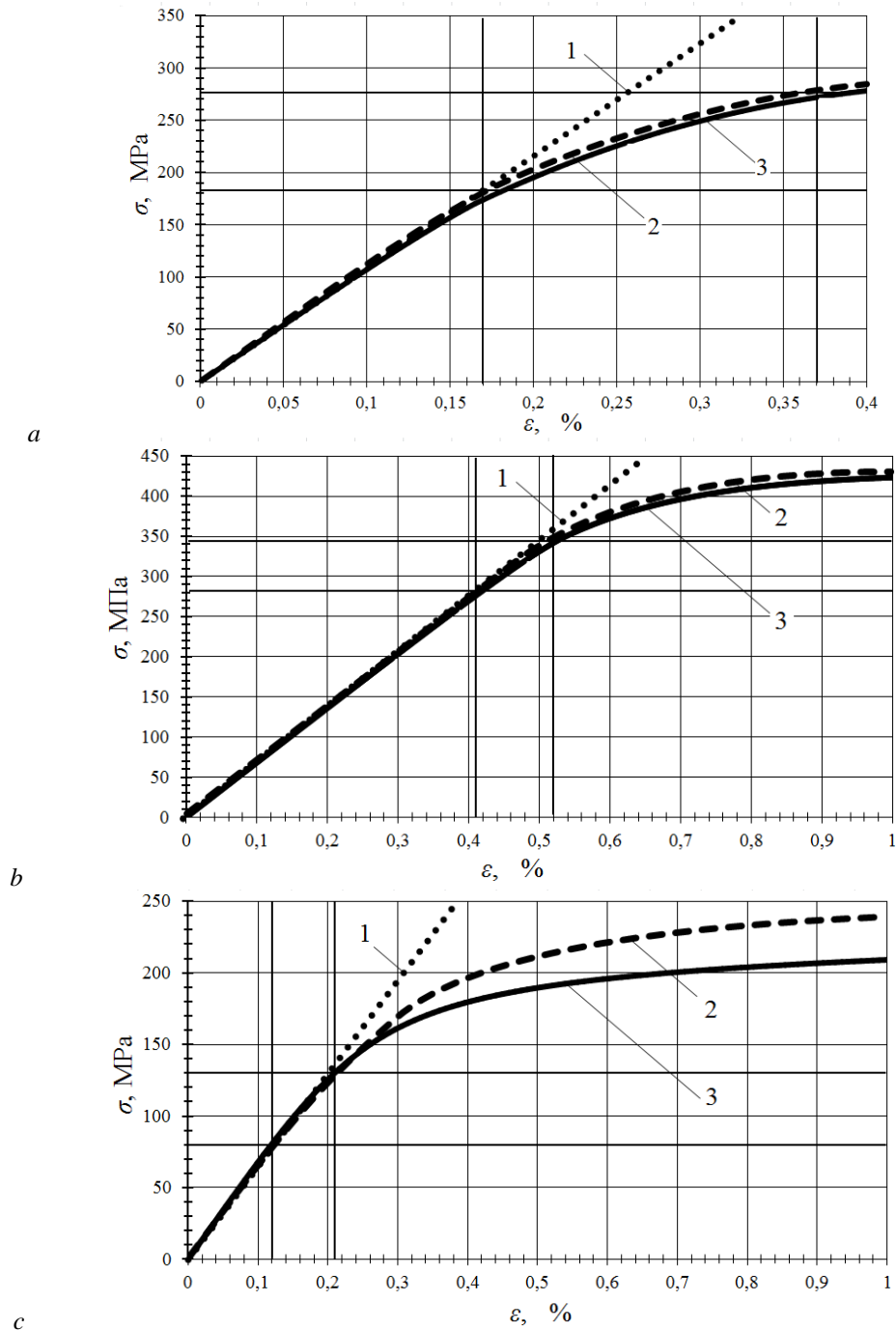

Figure 2: Dependence of stresses on strains under quasi-static tension: a – ferrite plastic material; b – brittle aluminum material; c – powder-reinforced composite based on aluminium; 1 – Hooke's law; 2 – experiment; 3 – simulation using the probabilistic approach

As it can be seen from Fig. 3, c, in this case for the composite there is no second part of graphs, which is typical for the both previous cases, where $\dot{\varepsilon}_{eq}^{p}$ exceeds $\dot{\varepsilon}_{eq}^{d}$. Consequently, in the whole considered range of strains, the

Vyacheslav Astanin, Oleksii Olefir, Ganna Shchegel, Andrii Olefir

deformation is of principally another nature, being brittle in this case. This theoretical conclusion, obtained solely on the basis of the probabilistic modeling, is confirmed by experimental data. It turns out that according to figure 8 in [13], microphotographs clearly indicate strands of plastic deformation on the boundaries of the destroyed surface in the case of aluminum and at the same time expressively brittle character without such strands in the case of reinforced with particles of aluminum composite.
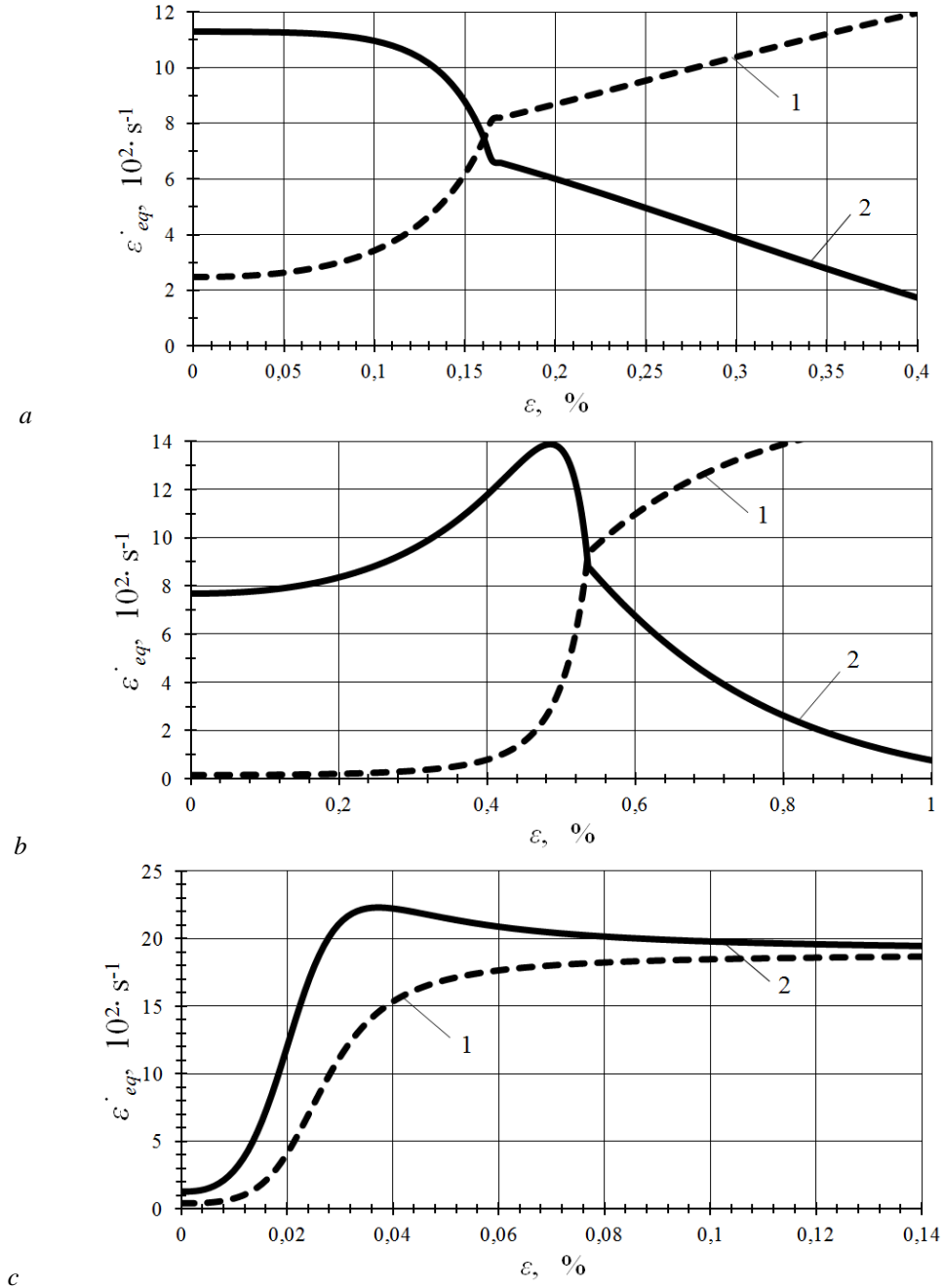

Figure 3: Dependences of equivalent strain rates of plastic $\dot{\varepsilon}_{eq}^{p}$ (1) and diffuse $\dot{\varepsilon}_{eq}^{d}$ (2) deformations on strain ε : a – ferrite plastic material; b – brittle aluminum material; c – powder-reinforced composite based on aluminium

6. Conclusions

A probabilistic approach to deformation and damage modeling of composite materials is proposed. It is based on the principle of calculating probabilities of destruction and restoration of force bonds between material structural elements, taking into account the frequency characteristics of these processes, as well as the corresponding

equivalent strain rates of plastic and diffuse deformations as parameters, on the basis of which the refined thermodynamic calculation of the deformation process is done. The carried out study of stress-strain dependencies of three structural materials, namely two metal alloys with a minimum amount of structural inclusions, and also a reinforced with silicon carbide particles composite on the basis of a metal matrix, showed the principal applicability of the proposed probabilistic model.

The advantages of the developed probabilistic model are the possibility of practically accurate prediction of strain values, at which a transition from predominantly elastic to predominantly plastic, or ductile, deformation takes place, as well as obtaining a fundamental answer to the question whether plastic deformation is going to occur at all.

Thus, the probabilistic model makes it possible at the early stage of simulation to predict not only the stress-strain dependence, but also the accompanying phenomenological phenomena, namely, if a deviation of this dependence from the Hooke's law is due to irreversible plastic deformations or, conversely, brittle damage, that is, the formation of microcracks, while other sites retain their initial intact internal structure. The first case is realized provided that the equivalent strain rate of plastic deformation exceeds the equivalent strain rate of diffuse deformation. The case of brittle damage is realized under opposite condition.

In addition, characteristic conditions have been revealed, which indicate weather random factors of the presence of local structural inhomogeneities in the material start playing the key role during the deformation and damage process. Such the case is then characterized with significant scattering of experimental values obtained in tests. Such the phenomenon is observed under conditions when the equivalent strain rate of diffuse and plastic deformations takes similar values. Therefore the physical processes of destruction and restoration of bonds allow with practically close probability the formation of both irreversible transverse gaps as cracks and also tangential sliding of the material layers as the mechanism of plastic deformation. Only under such condition the real material behavior is predominated by solely random factors of structural imperfections.

References

1. Hu J. Stress analysis and damage evolution in individual plies of notched composite laminates subjected to in-plane loads / J. Hu, K. Zhang, H. Cheng, P. Liu, P. Zou, D. Song // Chin. J. Aeronaut. – 2017. – vol. 30. – № 1. – p. 447-460.

2. Crookston J.J. Prediction of elastic behaviour and initial failure of textile composites / J.J. Crookston // Dissertation. – The Univ. of Nottingham. – 2004. – 217 p.

3. Paepegem W.Van Modelling damage and permanent strain in fibre-reinforced composites under in-plane fatigue loading / W. Van Paepegem, J. Degrieck // Compos. Sci. Technol. – 2003. – vol. 63. – № 5. – p. 677-694.

4. Li N. Micro-macro FE modeling of damage evolution in laminated composite plates subjected to low velocity impact / N. Li, P.H. Chen // Compos. Struct. – 2016. – vol. 147. – p. 111–121.

5. Astanin V.V. Impact deformation and fracture of hybrid composite materials / V.V. Astanin, G.O. Shchegel // Strength Mater. – 2011. – vol. 43. – № 6. – p. 615-627.

6. Tohei T. Debye temperature and stiffness of carbon and boron nitride polymorphs from first principles calculations / T. Tohei, A. Kuwabara, F. Oba, I. Tanaka // Phys. Rev. B: Condens. Matter. – 2006. – № 73(6). – p. 643041-643047.

7. Astanin V.V. Peculiarities of impact damage of textile-reinforced composite materials under high and low impact speeds (in Ukrainian) / V.V. Astanin, O.I. Olefir, G.O. Shchegel, A.O. Olefir // Technol. Syst. – 2016. – № 1(74). – p. 34-45.

8. Astanin V.V. Numerical simulation of high-speed impact of net-reinforced flexible composites (in Ukrainian) / V.V. Astanin, O.I. Olefir, G.O. Shchegel, A.O. Olefir // Technol. Syst. – 2014. – № 4(69). – p. 22-29.

9. Astanin V.V. Probabilistic modeling of physical damage processes of fiber-reinforced composite plates under dynamic loading / V.V. Astanin, G.O. Shchegel // Sci. J. of the Ternopil Nat. Techn. Univ. (Mech. and Material Sci.). – 2016. – № 2(82). – c. 7-22.

10. Astanin V.V. Numerical realization of probabilistic model of composite material taking into account the damage evolution at high impact velocities / V.V. Astanin, G.O. Shchegel // Sci. J. of the Ternopil Nat. Techn. Univ. (Mech. and Material Sci.). – 2016. – № 3(83). – c. 16-27.

11. Atlas of stress-strain curves. 2nd ed. / Materials Park: ASM Int., 2002. – 816 p.

12. (2016, Nov.) The engineering toolbox. Resources, tools and basic information for engineering and design of technical applications. [Online]. http://www.engineeringtoolbox.com/young-modulus-d_417.html

13. Li Y. The mechanical response of an A359/SiCp MMC and the A359 aluminum matrix to dynamic shearing deformations / Y. Li, K.T. Ramesh, E.S.C. Chin // Mater. Sci. Eng., A. – 2004. – vol. 382. – № 1. – p. 162-170.

Vyacheslav Astanin, Oleksii Olefir, Ganna Shchegel, Andrii Olefir

14. Astanin V.V. Probability approach to the problem of impact-induced damage simulation of composite plates / V.V. Astanin, A.A. Shchegel' // Strength Mater. – 2017. – vol. 49. – № 2. – p. 280-291.

15. Astanin V.V. Numerical simulation of stresses and deformations of simple composite elements using probabilistic approach (in Ukrainian) / V.V. Astanin, O.I. Olefir, G.O. Shchegel, A.O. Olefir // Technol. Syst. – 2017. – № 1(78). – p. 41-52.

16. Astanin V. Experimental and probabilistic numerical modelling of impact of fiber-reinforced composites at high and low velocitieses / V. Astanin, G. Shchegel // Sci. J. of the Ternopil Nat. Techn. Univ. (Mechanics and Materials Science). – 2016. – № 4(84). – p. 7-22.

17. The predictive capability of failure mode concept-based strength criteria for multidirectional laminates / Failure criteria in fibre-reinforced-polymer composites (The World-Wide Failure Exercise) / R.G. Cuntze, A. Freund. – M.J. Hinton, P.D. Soden, A.S. Kaddour, ed. – Amst.: Elsevier, 2004. – p. 429-489.

18. Damage and failure of aerospace composites / Structural health monitoring of aerospace composites / V. Giurgiutiu. – V. Giurgiutiu, ed. – N.Y.: Elsevier Inc. Acad. Press, 2016. – p. 125-175.

19. Gude M. Damage evolution of novel 3D textile-reinforced composites under fatigue loading conditions / M. Gude, W. Hufenbach, I. Koch // Compos. Sci. Technol. – 2010. – vol. 70. – № 1. – p. 186-192.

20. Gariboldi E. Damage mechanisms at room and high temperature in notched specimens of Al6061/Al2O3 particulate composites / E. Gariboldi, A. Lo Conte // Compos. Sci. Technol. – 2008. – vol. 68. – № 1. – p. 260-267.

21. Handbook of mathematical functions / M. Abramowitz, I.A. Stegun, ed. – N.Y.: Dover Publ. Inc., 1965. – 1046 p.

22. Laurendeau N.M. Statistical thermodynamics / N. M. Laurendeau. – N.Y.: Cambridge Univ. Press, 2005. – 448 p.

23. Kittel Ch. Introduction to solid state physics / Ch. Kittel. – St. Johnson, ed. – N.Y.: John Wiley & Sons, 2005. – 680 p.

24. Huang K. Statistical mechanics / K. Huang. – N.Y.: John Wiley & Sons, 1987. – 506 p.