Diagnostic features of relief formations on the nanostructured titanium VT1-0 surface after laser shock-wave treatment

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Abstract. A new class of diagnostic features for conducting morphological analysis of relief formations induced by laser shock-wave treatment on the surface of the nanostructured titanium VT1-0 alloy is proposed. They are the coefficients of series expansions of statistical estimates for the orthogonal basis of Chebyshev, Laguerre, Kravchuk discrete polynomials and trigonometric functions. Based on the criterion of the minimum number of the diagnostic features in the above-mentioned bases, the Chebyshev one was selected as the most appropriate to solve this problem.

1. Introduction

The relationship between structural features of materials and constructions with their physical-mechanical properties, particularly strain resistance, can be established on the basis of the concept of structural levels of deformation, which belongs to the area covered by the physical mesomechanics of materials [1].

Practical applications of this approach are of importance when analyzing complex deformation processes that take place in structure-sensitive materials and constructions [2]. In doing so the material surface is considered as an indicator to characterize processes of damage accumulation in the form of shear and rotational displacements of elementary structural elements – grains, or rarely their conglomerates. Since this process possesses an expressed stage and a monotonic pattern, it makes it possible to use the data on the surface strain induced relief to evaluate a (diagnostic) state of the object. Let us consider the behavior of the surface characteristics of the material in more detail [3].

The surface is treated as a complex, hierarchically organized system that under loading induced accumulation of micro-damages evolves and adapts to the force effect [4-6]. This self-organization results in the formation of strain induced relief which might be taken as an informative parameter of the system mechanical state. There are some literature data on attempts to propose a mathematical description of the relief formations. They allow us to establish the relationship between deformation processes that develop at the macro-, meso- and microscale levels [7-9]. Also, a number of papers devoted to the experimental analysis of the surfaces state in a number of materials under static, cyclic and shock-wave loading are available. However, in general, mathematical processing of the results and particularly procedures of their numerical automated analysis requires their further development. Design of modern systems for the processing and simulation of cyclic attributes of the relief formation...
allows automating and substantially intensifying the process of their analysis, diagnosis and prognosis, as well as opens the possibility of carrying out computer simulations during their modeling.

The aim of this study is to substantiate the required minimum set of diagnostic parameters that are sensitive to the relief formation process and might be employed as the informative features/attributes for automated diagnostic systems.

2. Physical reasoning for relief formation attributes analysis
Plastic deformation at the mesoscale level in the surface layers of nanostructured materials is developed with low energy dissipation. It is this fact that allows one to reveal nonlinear waves of localized plastic flow in nanostructured surface layers [10]. Regularities of nonlinear wave formation are associated with an ordered distribution of stresses and self-organization which take place in the nanostructured material under loading.

The data obtained with the use of the interferential profilometer ‘Micron-alpha’ were employed to investigate micro-localizations of relief formations on the surface of the nanostructured VT1-0 titanium after laser shock-wave treatment. The obtained experimental data make it possible to reveal distribution of relief formations that exhibit a "chessboard" pattern in two-dimensional observation where the regions experiencing compressive stress are alternated with tensile stressed ones [1, 2]. Stress relaxation can take place through the processes of heat and mass transfer being initiated in the tensioned regions towards the compressed ones. In so doing, a folded relief is formed in places where the maximum compressive stresses are reached.

Nanostructured titanium specimens were subjected to laser shock-wave treatment in various environments: air, water and ink. Specimens with the 80×80×5 mm gauge length were treated with the use of the GOS-1001 laser with the LiF gate in a Q-switched mode. It is suggested that the material surface "feels" deformation manifestations that are accompanied by the generation of deformation fields which spatial structure reflects the functional state of the material. The using of the non-contact profilometry of high resolution makes it possible to obtain a clear numerical characteristic of the surface state being covered with strain induced relief formations. The data obtained were regarded as the attributes which can be analyzed using statistical methods [11]. This predetermines the fundamental possibility of increasing the accuracy, informativeness of automated (computer-aided) processing of such attributes and determination of the surface state condition through the analysis of the relief formations. This approach can ensure standardization of automated processing and simulation of relief formation attributes at various stages of structures life-time assessment, and improve the accuracy and completeness of the technical diagnosis resulting from the use of the similar diagnostic features.

3. Methodological approach
The estimates of the obtained probability characteristics [9] might be used as diagnostic features. However, they possess the substantial drawback – a large number of samples that are necessary to be set (samples of the estimate for the expectation and the variance). This makes it difficult to use them in constructing training sets in the systems for analysis of the diagnostic attributes.

In order to reduce the dimension of the diagnostic feature space under analysis of the obtained probability estimates, it is suggested to use the coefficients of orthogonal representation estimates of the mathematical expectation and the variance in the series of orthogonal bases as the diagnostic attributes. If a system of orthonormal discrete functions is given as \( \{ \psi_n(l), n \in \mathbb{Z}, l = 0, \ldots, L \} \), discrete function \( f(l), l = 0, \ldots, L \) can be written as a series of

\[
 f(l) = \sum_{n=0}^{\infty} c_n \cdot \psi_n(l),
\]

\[
 c_n = \sum_{l=0}^{L} f(l) \cdot \psi_n(l) \cdot \rho(l),
\]

where \( c_n \) – the coefficients of the series; \( \rho(l) \) – the weight function which selection depends upon
the type of the approximating function: the weight function should reach a maximum in the area where
the best approximation is required.

Complex \( \{c_n, \ n \in \mathbb{Z}\} \) is called function range \( f(l), \ l=0,L \) in orthonormal basis
\( \{\psi_n(l), \ n \in \mathbb{Z}, \ l=0,L\} \).

It is known that the same function can be expanded in a series of different orthonormal bases.
Let us represent function \( f(l), \ l=0,L \) as a series (2) as well as one in the basis of other orthonormal
functions \( \{\varphi_k(l), \ k \in \mathbb{Z}, \ l=0,L\} \)

\[
f(l) = \sum_{k=0}^{\infty} d_k \cdot \varphi_k(l),
\]
where \( d_k \) – the serial coefficient.

Let us multiply both sides (1) by \( \varphi_k(l) \) and sum over \( l \), where function \( f(l), \ l=0,L \) is given:

\[
\sum_l f(l) \cdot \varphi_k(l) = \sum_l \sum_{n=0}^{\infty} c_n \cdot \psi_n(l) \cdot \varphi_k(l) = \sum_{n=0}^{\infty} c_n \sum_l \psi_n(l) \cdot \varphi_k(l).
\]

The left side of this equation is the \( k \)-th coefficient of \( d_k \) of the normalized number for function
\( f(l), \ l=0,L \) while the sum of the right side (denoted by \( \Psi_{nk} \)) is a ratio of the same series for basic
functions \( \psi_n(l) \). Here,

\[
d_k = \sum_{k=0}^{\infty} c_n \cdot \Psi_{nk}.
\]

Coefficients \( \Psi_{nk} \) are independent of \( f(l) \). Thus, expression (4) establishes a relationship between the
spectra of expansion coefficients in series of function \( f(l) \) in different orthogonal bases.

Basic functions \( \{\psi_n(l), \ n \in \mathbb{Z}, \ l=0,L\} \) can possess quite complex spectrum at their expansion in
a series over the system of other orthogonal functions \( \{\varphi_k(l), \ k \in \mathbb{Z}, \ l=0,L\} \).

This proves the possibility of a system of basic functions to exist among certain systems of basic
ones that allow approximating function \( f(l), \ l=0,L \) with the same accuracy by the smallest number of coefficients in comparison with all other terms of this set.

A study on decomposition of different assessments of probability characteristics for variety of orthogonal bases was conducted. Within this research, we have limited it by the expansions of only a few orthogonal bases.

The most well-known and widespread polynomials with well-studied properties of an orthogonal
basis are discrete argument polynomials of Chebyshev, Kravchuk, Laguerre [12], and discrete
trigonometric functions. First, we have to determine the selection criteria for the orthogonal functions
system in which a series expansion will be carried out being based on the statistical processing
assessment results of expectation of the relief under analysis. In doing so, the criterion based on the
minimum amount of the first coefficients of the orthogonal series in case of their equal percentage
contribution to the total energy of the obtained probabilistic assessments was used. It is the so-called
discrete energy criterion.
The expansion of the expectation and the variance by the series for the four above-mentioned orthogonal bases was carried out. It is based on the criterion of a minimum number of the series coefficients, which contribute at least 95% to the total energy of the signal. It was found that the fewest number of coefficients is used during the expansion in series by Chebyshev orthogonal polynomials.

Thus, the coefficients of Chebyshev series are encouraged to use as the diagnostic features during the diagnostic evaluation of probability characteristics. The expectation estimates which were expanded in series by the selected polynomials is shown in Figure 1, while their results – in Figures 2, 3, 4.

**Figure 1.** Estimation of the expectation for the relief formations width on the surface of nanostructured titanium after laser shock-wave influence in air [9].

**Figure 2.** Expansion of estimates in series of trigonometric functions; two-component.

**Figure 3.** Expansion of estimates in Laguerre (a) and Chebyshev (b) series.

**Figure 4.** Expansion of estimates in Kravchuk series.
4. Discussion
Let us note that "the relief segments" formed on the surface of the material after the treatment are not equal. This is related to the local heterogeneity of the metal melting, crystallization and evaporation processes to take place on the material surface under laser irradiation [13]. Development of these processes depends on the pressure and duration of the shock pulse which are crucial during ordered relief formation in the area under modification.

The above-stated features of the processing of the analyzed cyclic signal allow us to cover all modes of nanostructured titanium modification. In doing so, they might be considered as a particular case in the framework of a united theoretical-methodological approach as well as take into account the wide range of possible cyclic attributes (to reflect the recurrence of signals in the structure) and the substantial structural differences during relief variation. As a result of the expansion and the analysis, the block diagram is given in Fig. 5 which shows the percentage energy contribution of two series factors of the studied orthogonal polynomials. The greatest energy contribution is made by two coefficients of the Chebyshev series — 99.45 %, while the coefficients of the series of trigonometric functions are 99.56 %. However, in the case of the series expansion in the trigonometric functions, the four coefficients \((A_1, A_2, B_1, B_2)\) are to be considered. In order to minimize the number of the diagnostic features, only two coefficients of Chebyshev series were selected.

![Figure 5](image)

**Figure 5.** The block-diagram illustrating series expansion in orthogonal bases.

A series of experiments in which the expectation estimates were expanded in series of orthogonal Chebyshev, Kravchuk, Laguerre bases by the discrete trigonometric functions has been conducted. On the basis of the criterion of the minimum number of terms in the series that bring the total signal energy contribution not less than 95%, it is proposed to use the coefficients of the Chebyshev series of discrete argument as a diagnostic attributes.

The proposed mathematical approaches can be used to develop special software aimed at running surface diagnostics of the nanostructured titanium implants after the high-energy treatment [14]. The use of this approach allows us not only to develop an express method for diagnostics, but also to predict the mechanical state of the surface layer of modified materials.

5. Conclusion
A new class of diagnostic attributes in the form of expansion coefficients of statistical estimates (expectation estimates) of relief formation in a series of Chebyshev orthogonal polynomials for the problem of morphological analysis under different modes of the laser shock-wave treatment has been proposed. The resulting expectation estimates can serve as a physical-mechanical basis for further diagnosis of the mechanical state of these materials surface layer through the analysis of the local region subjected to various types of the treatment/modification.
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