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Software Modeling Environment for Solving Problems of Structurally Inhomogeneous Materials

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Abstract. In this scientific study, the main properties of structurally inhomogeneous materials are predicted by computer modelling methods. The automatic combination of a scanning microscope and a program cell makes it possible to view the procedure in detail before and after etching with the necessary increase in resolution. Based on the results obtained, we constructed a graphical dependence of the particle sizes of 40 XH steel on the iterative process, and also studied in detail the procedure for the effect of different particle sizes on porosity. We modelled 2D and 3D drawings of the PRT–7 shaft part. We justified the predicted number of properties, in particular: porosity, particle shape, grain size, microstructure of the sample surface, pre-etching process, post-etching process, as well as the main advantages of the iterative process.

1 Introduction

Modern scientific and technological progress has always been, is, and will always be inextricably linked with the emergence of new ways of qualitative research of materials and products [1, 2]. Including with the specified and initial parameters, or with their own acquired unique (unusual) characteristics [3, 4]. This will allow creating and implementing new progressive and resource-saving technologies, as well as creating new equipment or improving it with a modern software environment [5, 6]. It should be noted that new materials also include porous materials, structurally inhomogeneous materials, and composites [7, 8]. Products made from such materials are used in modern technology of mechanical engineering, heat power, automotive industry, as well as in other branches of the national economy and not only [9, 10, 11]. The main stage of development of structurally inhomogeneous materials under study is their design, mathematical and computer modelling [12, 13]. It should be noted that real materials or powder mixtures usually have an inhomogeneous structure, which must be studied in detail [14]. The main aspects of the present concerning mathematical or computer modelling of materials, as well as their final operation (products-parts), taking into account the specified properties or completely new materials and obtaining new properties based on traditional approaches of mechanics [15, 16] or materials science [17, 18], in particular, in many cases are insufficiently studied [19]. In this case, it is necessary to use current methods for studying structurally inhomogeneous (heterogeneous) media. To a large extent, this refers to the main stages of dynamic deformation [20], which have a number and process of creating heterogeneous structures of materials and changing their nature during the deformation process [21, 22]. Because the diversity and mutual influence of such effects as: phase transitions [23], chemical reactions of components [24, 25, 26], heat exchange of materials [27], capillary effects [28], diffusion and chaotic motion of particles [29], etc. on the one hand, and the circumstances in which these effects manifest themselves, on the other, leads to a certain disconnection of research in this area. Therefore, the general problem of quantifying the entire variety of the above-mentioned deformation processes of heterogeneous media, including in the applied aspect, cannot be considered definitively solved and requires further study. Thus, the software modelling environment for solving problems of structurally inhomogeneous materials is an urgent task and requires constant detailed research.

2 Main Part

The beginning of systematic research in the field of powder metallurgy was laid in the works [30]. The main ideas of studying powder components with partial intervention of computer modelling are justified in scientific works [31]. Initially, the discrete theory of bulk media was used, which is mainly used in mechanics. After that, the authors began to apply and use more complex theories, including phenomenological and structural-phenomenological [32]. It should be noted that in the framework of the first approach, information was mainly used, according to which the material is mainly deformed, which can only be represented in a plastic-compressible and isotropic form, which does not satisfy the entire system of equations from the theory of powder composite research. The materials [33] study environments that substantiate only the rheological characteristics of the material, which are determined under experimental conditions. The development of research in the field of plastic flow of non-compact materials using certain structurally inhomogeneous media and a structural-phenomenological approach is considered in scientific teams [34]. General characteristics and properties in this case are obtained from the analysis of individual elements of the structure and modelling of individual elements of the part is considered. The authors also proposed a model of a porous medium, which is depicted as a rigid frame saturated with the gas phase.

It should be noted that the proposed various models of porous media, which are directly performed by theoretical studies and confirmed by experimental data, are highlighted in the works [35, 36]. In this case, a large number of processes related to the formation of powder materials are highlighted, as well as their main regularities are established. However, with a large amount of research, the practical results of using parts (i.e., the final results of parts by modelling methods) are not fully taken into account. Materials [37] have developed a microscopic examination technology that allows us to establish the main patterns between the porosity and particle size of powders. The shape of heterogeneous components is also taken into account. At the same time, the software environment for modelling the studied materials is poorly covered, which would make it possible to obtain much more physical and mechanical properties. In the works [38, 39], the structure of samples made mainly of spherical particles of materials is presented, various interpolation dependencies are presented, and the error of occurrence that occurred at the initial stages of the study is justified. It should be noted that the authors of this study described too narrow a range of tasks. Because powder metallurgy occupies a special place among various methods of processing materials, since it allows you to obtain not only products of various shapes and purposes, but also to create fundamentally new materials with new physical and mechanical properties[40], which are sometimes very difficult or impossible to obtain in any other way. It should be noted that these materials can have a complex of a number of unique properties, as well as significantly improve the economic performance of any type of production. In particular, the possibility of manufacturing products directly from powders is important both from the point of view of the efficiency of the technology itself, and as a method for obtaining materials with specified or fundamentally new properties. Therefore, the development of a software modelling environment for solving problems of structurally inhomogeneous materials is an urgent task and requires constant research.

The aim of the work is to develop an application of the Smart-eye software environment for solving problems of modelling structurally inhomogeneous materials. Based on the results obtained, to study a number of properties of steel grade 40 HN, as well as to model 2D and 3D parts – shaft grade PRT-7.

Materials. The aim of the study was to obtain detailed information about the surface topography (micrography) of the test sample in the direct tunnel current mode of the scanning microscope, as well as in the mode of the developed Smart-eye software environment. It should be noted that the general scheme of the scanning microscope includes the main phenomenon of the quantum and mechanical tunnel effect, which consists in a large ability to apply the necessary resolution, which allows a high-quality study of particles, and also allows you to overcome potential barriers (i.e., the total energy of the powder particle). The main contribution to the application of the Smart-eye software environment and the scanning microscope is made by electrons with the highest energy, which are at high levels close to the E_F level. It should also be noted that in the DC mode of the scanning microscope, the value of the tunnel effect that is focused between the probe and the test sample is maintained by approaching and diverting the probe to the required distance, as well as the application of the software environment and its feedback system. A signal that examines the selected areas on a micrograph with the intervention of a microscope (figure 2 and figure 3) taken from channel *Z*, i.e. piezo drive. Surface topography is generally investigated by an alternative recording method that continuously reports major events and moments, as well as the problems that are detected during the study. In figure 1 a general view of the jumping microscope is presented with a detailed description of its main components.

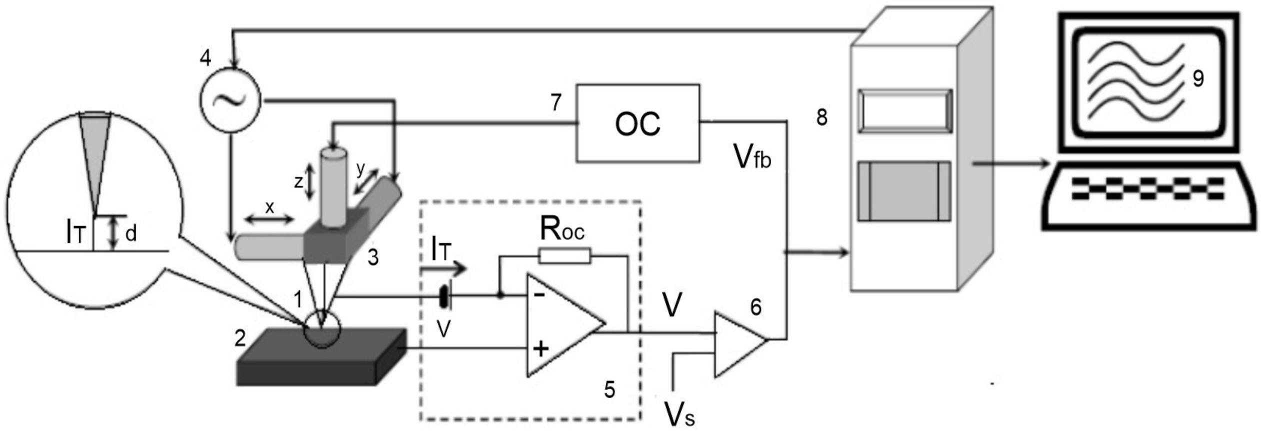

Fig. 1. General diagram of a scanning microscope, where: 1 – probe; 2 – sample; 3 – piezoelectric motors at *x*, *y*, *z* coordinates; 4 – data opening generator at *x* and *y* coordinates; 5 – sensor; 6 – compiler; 7 – feedback unit; 8 – computer; 9 – image at *x*, *y*, *z* coordinates (research results)

The proposed Smart-eye modelling complex in combination with the scanning microscope operation process is used to solve problems of structurally inhomogeneous materials mainly in the study of small, flat, and most problematic areas or areas of smooth surfaces or hard surfaces. The advantage of the complex is the constant work of feedback with the researcher. Also, the studied materials are constantly supported by the application of the software environment and record changes in the tunnel current of the scanning microscope as quickly as possible.

Tests. Using the Smart-eye software environment and a whole complex of scanning microscopes, the surface of material samples was examined. In Fig. 2 shows a micrograph of samples made of 40 XH grade steel before the etching process. And in Fig. 3 shows a micrograph of samples made of 40 XH grade steel after the etching procedure.

It should be noted that the study in both cases was conducted with a certain increase in resolution, which was equal to 700 × 800 dots per inch (i.e., 70 dpi and 80 dpi). This, in turn, allowed us to bring the experimental results of the iteration closer in detail to the correct statement. In Fig. 4 shows the graphical dependence of the particle sizes of 40 XH steel on the iterative process. This process (computer modelling) made it possible to record the most active particles of powders of heterogeneous materials, namely: d =10 mm, d = 15 mm and d = 40 mm. Based on the iterative process, we constructed the dependence of porosity on the particle size of 40 XH grade steel, which is shown in Fig. 5.

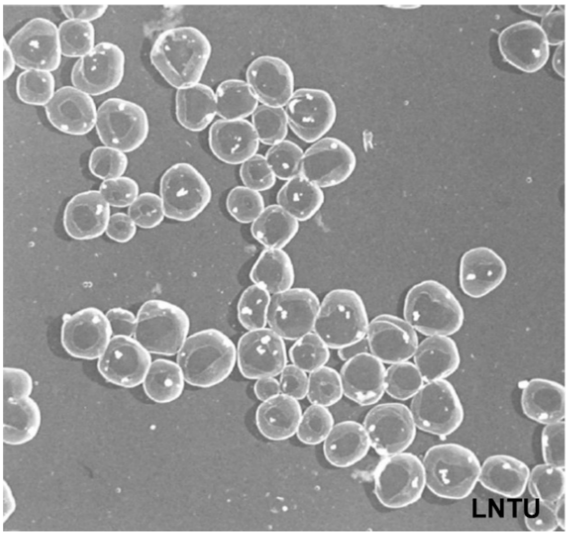

Fig. 2. Micrograph of samples made of 40 XH grade steel before the etching process

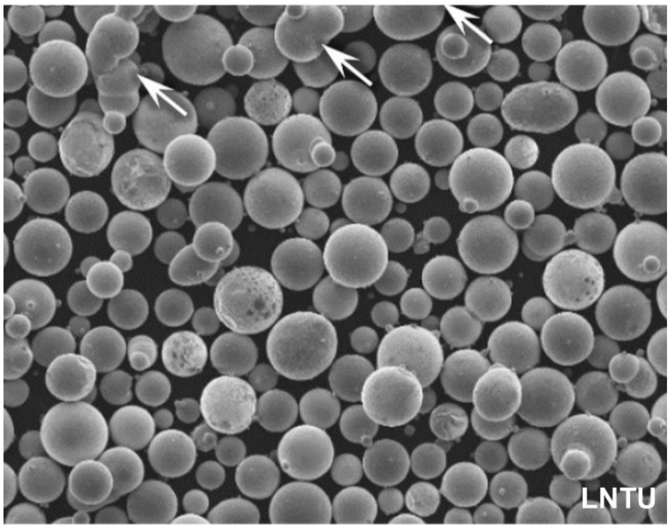

Fig. 3. Micrograph of 40 XH grade steel samples after etching procedure

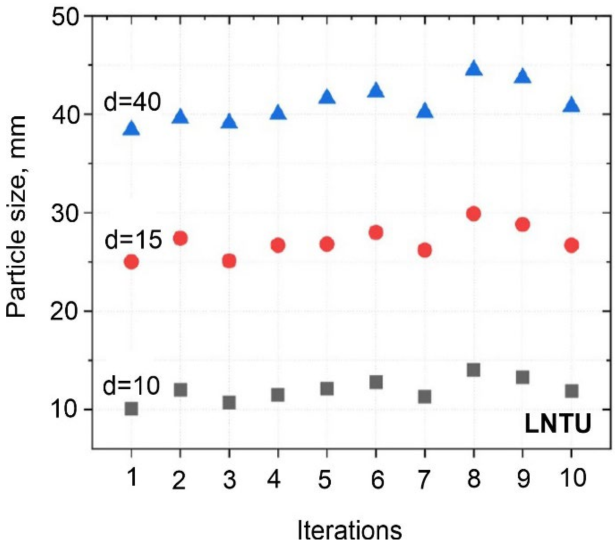

Fig. 4. Interpolation dependence of the 40 XH steel particle size on the iterative process

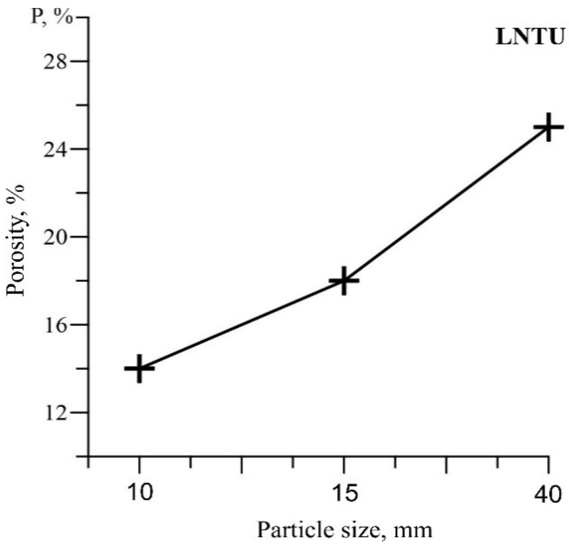

Fig. 5. Dependence of porosity on the particle size of steel grade 40 XH

From the dependency (Fig. 5) it follows that the porosity increases due to an increase in the particle size of inhomogeneous materials. This is due to poor compaction of powders of materials, which is easily solved by shaking (the process of vibration shaking). Basically, the particle size depends on the method of their manufacture and varies in this case from 10 mm to 40 mm. At the same time, we can firmly say that the results obtained make it possible to use this material – steel grade 40 XH for the manufacture of parts for various purposes. In Fig. 6 presents a 2D drawing of the part – shaft brand PRT-7.

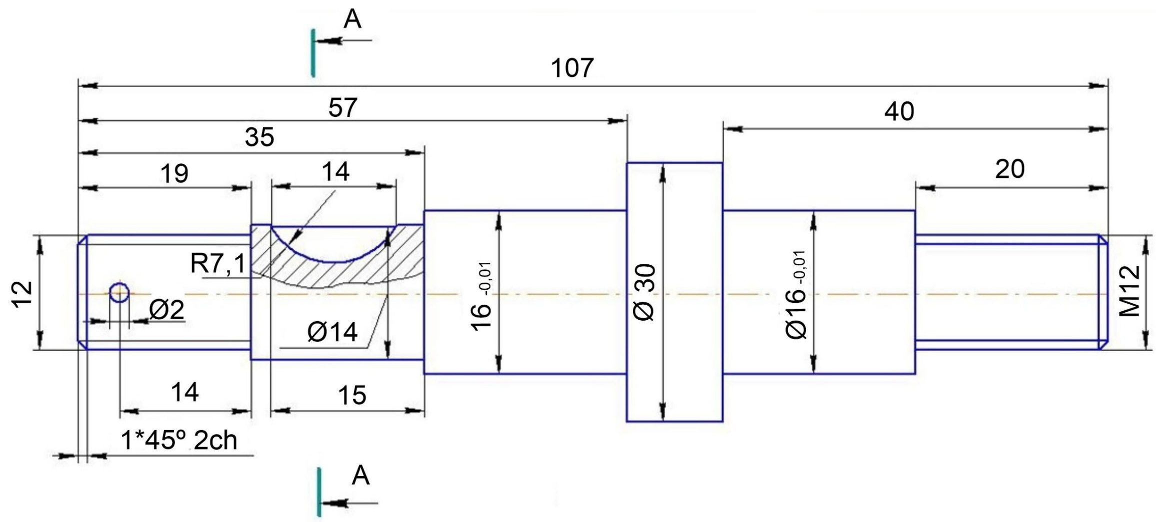

Fig. 6. 2D drawing of the part-shaft brand PRT-7

From a number of calculations, it follows that the proposed Smart-eye modelling complex with an automatic combination of a scanning microscope allows predicting individual physical and mechanical properties of steel grade 40 XH, which in this case is confirmed by practical application, namely the proposed part-the PRT – 7 Shaft. It should also be noted that the steel of the 40 XH grade studied by us has a number of properties (porosity, particle shape, grain size, microstructure of the surface of samples, the procedure of the process before and after etching, which allows you to study the structure from the inside, as well as the main advantages of the iterative process as a whole) and can also be used for another class of parts. For example: gear shaft, gear shaft, individual types of piston, rods, crankshafts, rings, rails, cam shafts, mandrels, bushings, spindles of different classes, various bolts, etc. In Fig. 7 presents a 3D drawing of the part – shaft brand PRT-7.

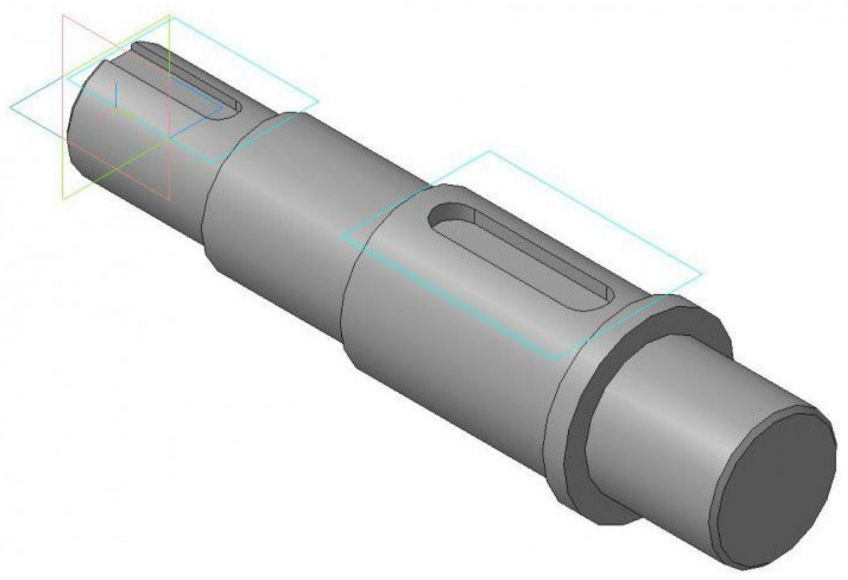

Fig. 7. 3D drawing of the part-shaft brand PRT-7

The conducted research fully meets the basic requirements of GOST 4543-2016 and GOST 4543-71 standards. This, in turn, fully meets the conditions of modern production and allows predicting such parameters as: strength of parts, accuracy and quality at a high level.

3 Conclusion

The proposed Smart-eye modelling software environment with an automatic combination of a scanning microscope allows you to solve a whole range of tasks, in particular:

1) investigation of the microstructure of samples, as well as their surface by optical and scanning microscopy methods;

2) investigation of the phase composition of materials, in particular chemical;

3) evaluation of mechanical and physical characteristics of structurally inhomogeneous materials in order to predict them.

The main advantages of the part we modelled – the PRT-7 haft with the proposed set of properties include:

1) it is characterized by a much higher load capacity at the specified specific interface parameters;

2) provides good alignment between the shaft and the hole;

3) provides an active possibility of any displacement, including axial displacement;

4) made of strong steel structurally inhomogeneous materials.

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