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APPLICATION OF THE FINITE ELEMENT METHOD FOR MODELING SOME MECHANICAL PROPERTIES OF POLYCRYSTALS

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Abstract. *Approaches for modelling of polycrystalline metals and alloys using single crystal fundamental characteristics are considered. An example of modelling is the simulation of the hardening curve of a high-strength titanium alloy. The simulation results have proved satisfactory for further use of this approach in determining other characteristics used in process calculations of forming.*

Keywords: simulation, polycrystalline metals and alloys, single crystal, finite element method, strain-stress curve, mechanical characteristics.

The mechanical properties of polycrystals and creation of their models can be obtained in two ways - the direct way, by study of full-scale specimens with the use of phenomenological theory of elasticity, plasticity and deformability and the calculation way, based on simulation, using the properties of single crystals and their interaction with each other under the influence of external loads. Until recently, implementation of the second way has been rather problematic, because such calculations required considerable computational resources, corresponding methodology and software. The first approach requires the large experimental base of research and therefore is both labour-intensive and expensive. At the same time, obtaining data on the behaviour of materials under new conditions usually requires setting up new experiments, which in addition to the above mentioned is not flexible and is costly. The second way is devoid of such disadvantages, as it uses the basic properties of single crystals for simulation of macro-characteristics of mechanical properties of polycrystalline samples. In this case, there is calculation error, however, in case of search for optimal solutions the second way is undoubtedly preferable. Also, using the second approach it is possible to simulate some mechanical properties even of materials which do not exist in the reality [1]. The most important characteristics used for practical calculations of polycrystalline material forming processes should be noted: Average Young's modulus, Shear modulus, Poisson's ratio, Hill's parameters, YTS, UTS, Relations true strain - true stress; Diagram of Bauschinger for anisotropic hardening; Diagram of plasticity etc. All of above are functions of temperature, chemical composition, technology of obtaining etc (microstructure, phase). Today's software [free software NEPER (https://neper.info/), FEpX (https://fepx.info/), DAMASK (https://damask.mpie.de/), commercial finite element software ABAQUS] and hardware already allow to implement the phenomenological approach quite effectively. The basic software used to investigate the mechanical properties of polycrystalline materials is Neper and FEpX. Neper was used as the basic program to prepare a geometric model of materials with a polycrystalline structure; FEpX was used to simulate the plastic properties of polycrystalline materials. The main focus has been on exploring the capabilities of FEpX and the theoretical basis of the models used in the program. A number of elasticity and plasticity characteristics, which are part of the model of the mechanical properties of the material, were investigated on their basis. The elastic properties of polycrystals are described using generalized Hooke's law and plasticity properties are described using models proposed by Garson [2] using Voce phenomenological models. It is concluded that the description of the plastic and elastic properties of crystals at the microlevel is phenomenological, i.e. the model constants are studied on the experimental research ground. In this case, a part of the experiments is rationally performed in an ad-initio simulation mode. For instance, such studies are important for polycrystalline magnetic materials with new chemical composition based on manganese, aluminium, nickel, copper and other materials.

For polycrystalline materials the most important characteristic for modelling different shaping processes is the stress-strain curves. These relationships can be obtained using a simulation with FEpX by loading of a cubic specimen with unit dimensions. Verification of the simulation results was done with using known literature data of polycrystalline materials (copper, high-strength titanium alloy Ti-6Al-4V [3], as well as the experimental data obtained in our earlier studies [4]. A satisfactory correspondence between the calculated curves and the experimental data R_{adj} = 0,95 has been obtained. One of the important results of these studies was the study of influence of particular model parameters (Garson17) on plasticity characteristics. Thus the number of crystal plasticity parameters for titanium alloy may be taken as constants (in particular, fixed-state strain rate scaling, saturation strength rate scaling coefficient and power on modified Voce hardening term equal 1, saturation strength rate scaling exponent equal 0,01).

Another important aspect of modelling is the calculation of residual thermal stresses in polycrystalline solids, which in some cases can achieve values that have a significant impact on their functional performance. Such materials include, for example, permanent magnetic materials based on neodymium-iron-boron. Using FEM simulation it is possible to obtain reliable values of the stress-strain state after heat treatment, which in turn is the basis for further optimization of the material structure.

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ЗАСТОСУВАННЯ МЕТОДУ СКІНЧЕННИХ ЕЛЕМЕНТІВ У МОДЕЛЮВАННІ ДЕЯКИХ МЕХАНІЧНИХ ХАРАКТЕРИСТИК ПОЛІКРИСТАЛІВ

Анотація. *Розглянуто підходи до моделювання полікристалічних металів і сплавів з використанням фундаментальних характеристик монокристалів. Прикладом такого моделювання є розрахунок кривої зміцнення високоміцного титанового сплаву. Результати симуляції виявилися задовільними для подальшого використання цього підходу при визначенні інших характеристик, що використовуються в технологічних розрахунках процесів формоутворення.*

Ключові слова: моделювання, полікристалічні метали і сплави, монокристал, метод скінченних елементів, крива "деформація-напруження", механічні характеристики

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