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MODELLING OF STRAIN-STRESS CURVE OF POLYCRYSTALLINE MATERIALS BY THE FINITE ELEMENT METHOD

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Abstract

The idea of developing methods and methodology for calculating macrocharacteristics of technological properties of polycrystalline materials based on the characteristics of single crystals is suggested. A study of modern software that implements the finite element method for modelling the behavior of polycrystalline materials in the elastic and plastic regions is made. The strain-stress curve of a titanium alloy is modelled, and a conclusion is made about the rational modes of modelling and the acceptable accuracy of the results of modelling and experimental tests.

Keywords: modelling, polycrystalline materials, crystal, finite element method, strain-stress curve, mechanical characteristics, deformation.

Анотація

Висунута ідея щодо розвитку методів і методології розрахунку макрохарактеристик технологічних властивостей полікристалічних матеріалів на основі характеристик одиничних кристалів. Зроблено огляд сучасного програмного забезпечення, що реалізує метод кінцевих елементів для моделювання поведінки полікристалічних матеріалів в пружні та пластичні областях. Здійснено моделювання кривої течії титанового сплаву, зроблено висновок про раціональні режими моделювання та прийнятну точність результатів моделювання та експериментальних випробовувань.

Ключові слова: моделювання, полікристалічні матеріали, кристал, метод скінченних елементів, крива течії, механічні характеристики, деформування.

Introduction

Most construction materials have polycrystalline structure due to the nature of the material itself and the production technology. For engineering calculations, it is necessary to know the mechanical properties of a material, which include both standard engineering (elasticity, strength, ductility) and fundamental characteristics (flow and plasticity diagrams, stability curves). Today most of these characteristics are obtained via direct (probably destructive) tests, allowing to receive model parameters and material charts in the framework of the accepted phenomenological theory [1]. The inflexibility and high cost of this approach are its significant disadvantages. On the other hand, computer simulation of the mechanical properties of polycrystalline materials is a promising modern research trend [2]. Today's software [free software NEPER (https://neper.info/), FEpX (https://fepx.info/), DAMASK (https://damask.mpie.de/), commercial finite element software ABAQUS (CPFEM)] and hardware already allow to implement the phenomenological approach quite effectively. The study of polyfunctional materials often focuses on only one technological property. However, other properties such mechanical characteristics may strongly influence the figure of merit.

Results

Mechanical properties of polycrystals are still most often used in the form of well-known standard characteristics: these are basic engineering characteristics (elasticity characteristics in the form of Young's modulus, Poisson's coefficient; strength characteristics in the form of tensile strength, yield strength, plasticity, hardness, etc.) and special technological characteristics. However, in fundamental theories of elasticity, plasticity and deformability, the mechanical manifestations of bodies are based on the characteristics of elasticity (tensor of elastic properties); characteristics of plastic flow (a set of parameters describing the surface of the plastic yield beginning and its evolution during time); limiting characteristics (a complex of parameters characterising the achievement of limiting states - the beginning of fracture, both brittle and plastic, plasticity diagrams, lost stability of deformation, etc.). Exactly these characteristics are used by modern software package (ANSYS, ABACUS, MSC Marc, LsDyna, Deform, etc.) to simulate elastic-plastic tasks underlying both the technological processes of production of parts and the working conditions.

For polycrystalline materials the most important characteristic for modelling different shaping processes is the stress-strain curves. These relationships can be obtained using FEpX, using a simulation of the loading process of a cubic specimen with unit dimensions. For verification of the simulation results known literature data of polycrystalline materials (copper, high-strength titanium alloy Ti-6Al-4V [1, 3]. A satisfactory correspondence between the calculated curves and the experimental data R_{adj} = 0,95 has been obtained (Fig.1). One of the important results of these studies was the study of influence of particular model parameters (Garson17) on plasticity characteristics. The hypothesis that some parameters of the models can be taken as constants for different materials has been proposed, which requires further verification.

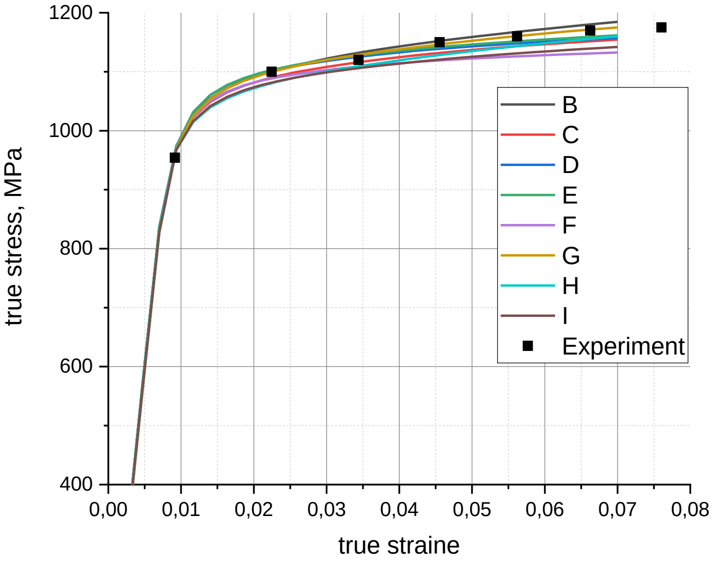
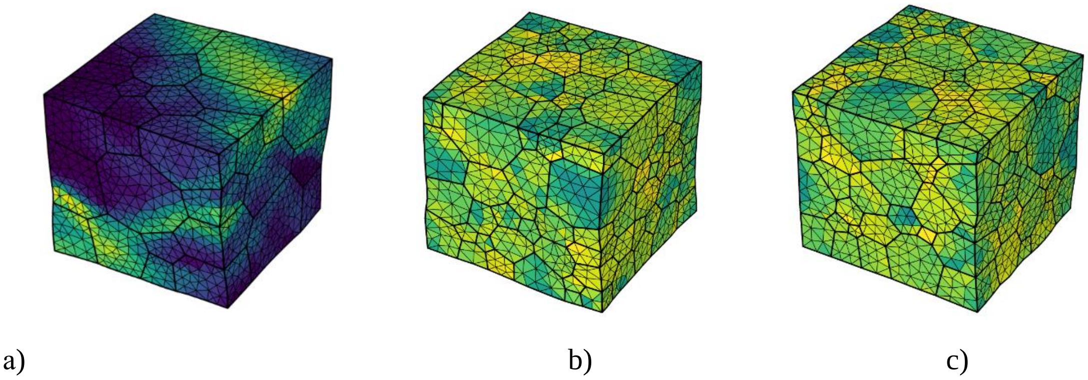


Fig. 1 – True strain-stress curves obtained experimentally [1] and by simulation (B-I) using different input data (low influencing parameters)

In total, more than 100 calculations with different simulation input data were carried out. In the course of the research, the optimum parameters for the tessellation procedure, finite elements mesh, assignment of boundary conditions according to real loading and experimental conditions, orientation of crystals in the element, target strain were established. The simulation time for the sample compression process was of the same order of magnitude (FEpX). It has been found that the tessellation parameters (grain orientation, number and shape) in geometric model preparation is a key factor influencing the final results (see fig. 2). In particular, a reasonable minimum number of grains per unit volume was found to be 200 if the orientation of the crystals is uniformly distributed on the volume. In this case tessellation method (parameter id) practically does not influence final results. When random orientation is used, the number of crystals has to be significantly higher, which is an irrational way of assigning such a parameter. Nevertheless, crystal orientation anisotropy parameters have to be taken into account in real process calculations where material texturing occurs. Significant decrease of the finite element size from the default one did not significantly change the computational results with a large increase of the computational time. For target plastic strain values of about 0.1 or more, there was almost always a problem with the convergence and stability of the calculation procedure, so the target strain was taken as 0.07.



a) b) c)

Fig. 2 – Optimal tessellation and deformed state of a single cube after achieving the target true compressive strain of 0.07 number of grains 200, "ori uniform", different "id" a-1, b-2, c-3

The stress-strain curves show slight dependence on loading conditions (tensile and compressive) and strain rate, and strong influence on boundary and loading conditions for the faces of a single cubic. Thus, the hypothesis of a single flow curve for polycrystalline materials was confirmed. It is shown that better results are obtained when simulating compression of the sample since the sample loses its stability during tensile stress with large deformations. The gripping conditions should be chosen as "minimum" which corresponds to the experimental situation when using effective lubrication of specimen faces during its compression in the die.

Concussions

A satisfactory correspondence between the calculated curves and the experimental data has been achieved. In the process of study optimal parameters of tessellation procedure (200 grains per unit volume), finite elements mesh, assignment of boundary conditions according to real conditions of loading and experiment, crystal orientation per volume (ori uniform), target strain (0.07) were determined. The stress-strain curves show slight dependence on loading conditions (tensile and compressive) and strain rate, and strong influence on boundary and loading conditions for the faces of a single cubic. The above results are important for further research in this field, as the time required to find optimal parameters for mathematical models of magnetic materials is significantly reduced.

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