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MULTILEVEL MODELING OF POLYCRYSTALLINE METALS MECHANICAL PROCESSING

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The internal structure of material substantially is changed in thermomechanical processing with attainment of plastic strain. It causes modifications of operational physical and mechanical properties. Therefore the actual problem is construction of materials mathematical models with a complex internal structure which can describe evolution of structure in thermomechanical processing and consider the influence of microstructure changes on the process parameters of macroscale level; these models can be using to improve manufacturing techniques of products.

In the last decades the multilevel models are proposed for solving this problem. These models are based on physical theories of plasticity, and it's structure explicitly comprises parameters, characterizing the internal structure, and evolution equations. Three main groups of models based on physical theories of plasticity can be presented depending on accepted hypothesis about the connection characteristics of different levels: statistical [1], self-consistent and direct models [2]. The application of self-consistent and direct models is related to extremely large computational efforts (the necessity of solving boundary value problem on the mesolevel), statistical models are mostly used for simulation of mechanical processing.

Original two and three-level statistical models of polycrystalline metals and alloys are offered. They contain the description of main mechanisms of inelastic deformation [3,4]: intragranular dislocation sliding, grain boundary sliding, twinning, breaking and fragmentation of grains, rotation of the crystallites lattice taking into account the inconsistency of dislocation motion in the neighboring crystallites. In these models connections between internal variables of different scale levels based on consistency of constitutive relations on levels is used [3], it allows to give description of geometric nonlinearity on macroscale level (specification of corotation derivative type of stress tensor).

Various integration schemes for differential relations of multilevel models are proposed, rising up consecutively on scale levels using different connections between internal variables on levels (without application of consistency conditions with using Jaumann derivative of stresses on macrolevel, with application of consistency conditions). Quaternions are applied for determining the orientations and rotations of moving coordinate systems on various scale levels. Computational time is decreased due to using parallel calculations.

The effective algorithm of using developed models for solving boundary value problems with finite element method is presented. Secants modules method is applied for introduction of nonlinear constitutive relations to finite element scheme (the choice is determined by implementation this method in the using package Abaqus). Analytic form for fourth-rank tensor of secant moduls is found. This tensor linearly relates stress and strain increments on macroscale level and depends on current values of internal variables: the critical stresses on slip systems in crystallites, the orientation of crystallographic coordinate systems and it's rotating velocity, stresses in crystallites.

The constitutive relations on macrolevel are not explicitly considered in many existing models [1,2], but the macroscale level is introduced during numerical implementation in finite element package Abaqus (the point of integration corresponds to crystallites sample), in which the Jaumann derivative of Cauchy stress tensor is used (the last one is automatically appointed in Abaqus for solving geometrially nonlinear problems). It violates the matching in multilevel mathematical model. It is shown that this approach may lead to physically incorrect results, in particular oscillations of stress tensor components on macrolevel are occured at the modelling simple shear (monotone stressing).

Simulation of some material processing during intense plastic deformation (pressing, forging, stamping and etc.) is performed with the developed software package. Changes of stress, strain and temperature fields, evolution of corresponding internal structure (forms, dimensions and orientations of crystallographic axes of polycrystals structural units – grains, subgrains, fragments), effective macroscopic elastic and plastic properties of polycrystalline materials through processing are determined. The obtained results satisfactorily match the experimental data.

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