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Modeling of grain refinement by cellular automata

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ABSTRACT

Prediction of microstructure evolution and properties of ultrafine-grained materials is one of the most significant problems in materials science. Cellular automata (CA) method is able for proper simulation of the microstructure evolution and can be used for evaluation of mechanical properties. The paper presents a new original application of cellular automata for modeling of grain refinement. CA take into account deformation, evolution of dislocation density and dislocation structures; and simulate microstructure evolution as grain refinement. Deformation of grains in polycrystalline materials depends on their crystallographic orientation, which is unique for every grain. It causes anisotropy of deformation in micro-scale. Joining CA with other methods (finite element, discrete element, crystal plasticity, etc.) improves accuracy of coupled phenomena modeling in micro- and macro-scale. Finite element method and crystal plasticity theory provide information for CA calculations. Grain refinement occurs in two stages: a creation of low-angle boundaries and their evolution into high-angle boundaries. Three CA models of low-angle boundaries creation were developed. They are described and discussed in the paper. Developed models can be used for study of processes of grain refinement, as well as can be a part of the system for modeling of microstructure evolution in the processes of solidification, hot and cold deformation and phase transformation. Examples presented in the paper are model application for processes with severe plastic deformation (SPD). Results of simulations of grain refinement during the accumulative roll-bonding (ARB) process and MAXStrain® technology are presented in the paper.

1. Introduction

The prediction of the microstructure and its digital representation in the micro-, meso- and macro-scale is one of the most important problems in materials science. Along with analytical and empirical models, Monte Carlo Potts models [1], the finite element method (FEM) based models [2], the phase field [3,4], multiphase-field [5] models, the front tracking method [6,7] and the vertex models [8] are used for modeling of microstructure evolution. But cellular automata (CA) models [9] occupy the first place among them. The CA applications for simulations of different phenomena are very important in the materials science, and their role is increasing. CA are used for modeling of crystallization (solidification) [10–14], dynamic and static recrystallization [15–18], phase transformation [17,19,20], cracks propagation [21], etc.

A new area of CA application is simulation of microstructure evolution for the processes with severe plastic deformation (SPD) [22–24] that provide grain refinement. In comparison with coarse structure, ultrafine-grained materials demonstrate high strength and low ductile-to-brittle transition temperature as well as high cycle and low cycle fatigue properties. The ultra-fine structure in metals and alloys can be obtained by using joint effects of severe plastic deformation and heat treatment [25]. In practice, a technology, where severe plastic deformation is carried out at lower temperature, is utilized. The conditions contribute to mechanical grain refinement, but do not allow recrystallization. The main factor in the process of grain refinement is an evolution of dislocation substructure. During the evolution, concurrent effects of different elements of the dislocation structure (interaction of dislocations with low- and high-angle boundaries, effects of boundaries and dislocation structure on hardening and so on) are changing.

Chemical composition and microstructure determine material properties. Difficulties in determination of material properties are connected with a lack of models and methods, which consider a contribution of particular elements of microstructure and transfer it from the microscale to the macro one. Additional sophistication is a shortage of methods, which allow to create a digital material representation and then analyze it.

Some disadvantage of CA is the fact that it does not give accurate determination of material properties explicitly. The structure obtained by CA is a discrete presentation, thus it is necessary to transform it into a form useful for numerical calculations, for example, by finite element method.

Microstructure evolution is pointedly three-dimensional, that is why 3D CA must be developed. Model takes into account theory of

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dislocation and plasticity of mono- and polycrystals, where main deformation mechanism is glide with consideration of kinds of crystal lattice, slip planes and slip directions. Appropriate connections between the main parameters of the deformation process (strain, strain rate and temperature) on the one hand and microstructure (substructure, high-angle boundaries, etc.) and material properties on the other hand are on a basis of proposed model.

Joining CA with FEM and other numerical methods improves accuracy of modeling of coupled phenomena during the forming processes in micro- and macro-scale. Deformation in micro-scale shows anisotropy. It is associated with the different crystallographic orientation of the grains in the polycrystalline material. That is why CA and FEM must be combined with crystal plasticity theory. Deformation in macro-scale is transferred to meso-scale, where representative volume contains several, score or hundreds grains, and then it is applied in micro-scale to each grain. Strain and strain rate are decomposed into the crystallographic slip directions. Dislocation evolution is considered for each direction separately. Dislocation structure in each grain evolves with different rate because orientation of every grain is unique. Evolution of substructure is an effect of generation and storage of dislocation in the subgrains and their boundaries. Disorientation angle between neighboring subgrains increase during the deformation because of subgrain rotation, which is a result of preferred storage of dislocations of the same signs on the subgrain boundaries. Creation of low-angle boundaries and their development into high-angle boundaries are simulated by CA on the base of calculations that are provided by finite element method and crystal plasticity theory.

The objective of the paper is development of three-dimensional frontal cellular automata (FCA) for modeling of the microstructure evolution during the process with severe plastic deformation and their implementation into the scheme for determination of material properties as well as into the system for modeling of technological processes.

2. General model

General block-scheme of joint model of microstructure evolution and mechanical properties for material with ultra-fine grains [22] is presented in Fig. 1. It includes models based on finite element methods (FEM I and FEM II), discrete element method (DEM), cellular automata (CA), as well as it uses crystal plasticity (CP) and modified KHL (Khan–Huan–Liang) model for calculation of microscopic flow stress. Because main objective of the paper is presentation of CA model, the other elements of general model are described very shortly.

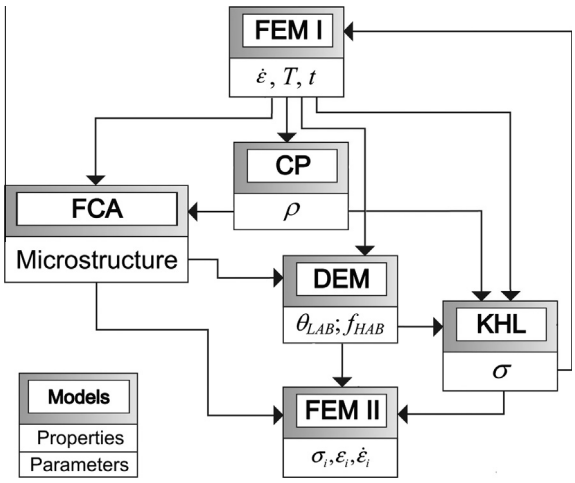

Fig. 1. Block-scheme of the calculation with proposed models and methods [22]. Models: FEM I – finite element model for macroscale, FEM II – finite element model for microscale, CP – crystal plasticity, FCA – frontal cellular automata, DEM – discrete element model, KHL – modified model of flow stress (Khan–Huan–Liang).

2.1. FEM I and FEM II

Finite element model FEM I is designed for modeling in the macro-scale with conventional and new model of flow stress [24]. At the beginning it uses simple conventional model and calculates trial deformation parameters. Then, after obtaining data from FEM II, FEM I repeats calculation with new dependences and rectifies parameters. Generally, arbitrary FEM code can be used as FEM I. It can depend on selected process with severe plastic deformation.

Model FEM II is designed for modeling of metal flow in microscale. It allows to take into account heterogeneity of deformation on the level of grains, especially inside them. It uses for calculation main principles of the crystal plasticity theory. Calculation results can be found elsewhere [24]. Abaqus Standard with combined submodeling technique and digital material representation approach [26] was used in the study for FEM II.

2.2. DEM

Discrete element model DEM is relatively new method. The main principles and applications can be found elsewhere [27]. DEM used in the present scheme (Fig. 1) is designed for modeling in the micro-scale. On the base of microstructure obtained from FCA each crystal is replaced by the set of spherical elements in view of crystallographic orientation and low-angle boundaries (LABs). The objective of the simulation is obtaining elements rotation upon the deformation. Spherical elements present dislocation cells, as nuclei of new fine structure. Rotation leads to the change of boundaries disorientation angle, and as result, LABs evolve to the high-angle boundaries.

2.3. Cristal plasticity (CP)

The present work is based on a crystal plasticity modeling, where the effects of deformation arise from the dislocation motion on active slip systems and from the distortion of the crystal lattice. Such a representation of material hardening is adequate for processes with severe plastic deformation.

Modeling of the evolution of dislocation density and substructure arrangement is the key factor in the analysis of nanocrystalline materials. In order to estimate quantitatively these processes, the variation of the dislocation cell size is very often implemented in the analysis [28]. The three main populations of dislocations form the substructure of metals and alloys with high stacking fault energy deformed with SPD technique: the immobile dislocation in the cells walls (ρ_w), the immobile dislocations in the cells interiors (ρ_i), and the mobile dislocations (ρ_m).

2.4. The macroscopic flow stress (KHL)

The macroscopic flow stress is calculated using a viscoplastic model that was proposed by Khan et al. [29]. However in the case of BCC structures subjected to severe plastic deformation with high microstructural and mechanical heterogeneity, where dislocation and substructure strengthening is significant, the better prediction of the flow stress gives modified version of the flow model presented by Dafalias [30].