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STUDY OF POLYCRYSTAL DEFORMATION USING CELLULAR AUTOMATA

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A computer model of a strain of polycrystals based on the concept of cellular automata is developed. The model allows one to investigate polycrystal as a multilevel hierarchical system and to study singularities of this system behavior depending on structure of material, strain mechanisms at the lower levels, program of loading and/or deformation at the upper level, temperature and other parameters.

1. Introduction

The traditional description of arbitrary strain of materials is mostly phenomenological. It is based upon the relationships connecting values of stress with the magnitude of residual strain; parameters of these relationships are determined in test experiments. For definite purposes connected mainly with the calculation of pressure treatment force conditions such description is quite satisfactory. However, as soon as there appear problems connected with the prediction of physical and mechanical properties of materials, with the research of stability of plastic deformation, fracture of materials, the phenomenological descriptions become unsuitable, as all indicated processes are essentially determined by a modification of an interior structure of material. For this reason per last 10–20 years there have been essential development of works lying on the joint of a mechanics and physics of a solid body. In these works the attempts of development of the deformable material models which take into account its microstructure are carried out. The known approaches of such kind belong to R. Hill, J.R.Rice [1], R.J.Asaro [2], Mokhel' A.N., Salganik L.R., Khristianovitch S.A. [3].

In the present work we propose a variant of such model based on the cellular automata [4,5]. The idea of cellular automata was independently introduced by John von Neuman and K.Tsuse at the end of 1940's. Both of them considered cellular automata as a universal computing environment for the construction of algorithms equivalent, by the indicative possibilities, to a Turing machine. The essence of cellular automata concept is that the area of a research is represented by a uniform grid, with each cell containing some bits of data; the time going forward by discrete steps, and the laws of a system behavior expressed by a unique set of rules (for example, small reference table) by which every cell at each step calculates its new state according to the state of its close neighbors. Thus, the laws of a system behavior have a local character. By means of numerical experiments the cellular automata allows one to study a behavior interdependence of the whole ensemble of cells on the local microscopic laws defining evolution of each cell. Therefore, the cellular automata represents a surprisingly appropriate tool for a computer research of a dependence of the response of

material for exterior action on mechanisms of plastic deformation.

Original authors' solution is the self-similar structure of cellular automata permitting at once to reflect in a model a fractal structure of real materials (it is known, for example, that the structure of actual steels represents fractal [6]). Besides, the self-similar structure can be adequately represented by methods of object-oriented programming for numerical experiments, that has allowed to use the latest developments of the programming languages providing high speed and economic distribution of computer RAM, obviousness of programming, possibility of easy modification to new mechanisms of strain and structure of materials.

2. Model description

2.1. Model of a polycrystal structure

According to modern views the deformable polycrystal has a multilevel hierarchical structure. There are 4 basic scale levels [7]:

– Microscopic (atomic) with a characteristic size l_{mic}=1÷30 a, where a – lattice constant;

– Mesoscopic (level of dislocational substructures) with a characteristic size l_{sub} = = 0.1÷3 μm;

– Structural (grain level) with a characteristic size l_{str} = 20÷200 μm;

– Macroscopic with a characteristic size l_{mac}>10 l_{str}.

Within the framework of mesoscopic and structural levels a polycrystal has a fractal structure [6], the distinctive feature of which is the self-similarity at the change of view level.

The described above structure of real polycrystal is simulated with the help of 3-D cellular structure. The cells can be simple and complex. The simple cells do not have an inner structure, the complicated cells consist of the simple and/or complicated ones. As a component, the complex cell may contain ones similar to itself. This allows to simulate fractal structures.

In the present work the complex cells having structure of cubic lattices and consisting of 27 (3×3×3) smaller cells (see fig. 1) are considered. In the general case other spatial structures and other amounts of components are possible.

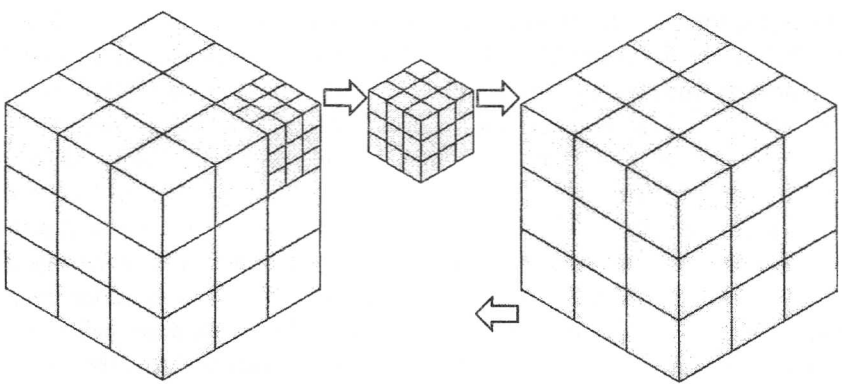

Fig. 1. Cellular automata structure

Let's consider the neighborhood of a cell which we understand as a group of its nearest neighbors. We assign a coordinate (m,n,k) to each cell that defines its position (m,n,k – integers from 1 up to 3). The central cell in fig. 1 has a coordinate (2,2,2), its neighborhood is formed by all remaining 26 cells. To define a neighborhood for boundary cells we assume that the system of cells in fig.1 is enclosed from different directions by ones similar to itself. This is the so-called periodic boundary condition. According to it the neighborhood of each cell out of 27 cells is formed by the remaining 26 cells.

Here we finish the exposition of a structure of our model and start reviewing its functioning. In summary we only state that the proposed model of a structure of polycrystal allows one to take into account a heterogeneity of a material at each scale level; to reflect a fractal nature of mesoscopic and structural levels; to describe easy interaction between processes happening at different scale levels.

2.2. Model of the stressed and strained state of polycrystals

The loaded polycrystal is characterized by inhomogeneous stressed and strained state (SSS). With the purpose of its description we will consider the stress tensor σ^n and plastic deformations tensor e_p^n for each cell from the structure suggested above. The index n in these terms specifies a level to which the considered cell belongs. It is assumed that the largest cell, which simulates representative volume of a macroscopic level, belongs to level 1; its component 27 cells belong to level 2; components of each from these 27 cells belong to level 3, etc. It is obvious that at the level with number n there are 27^{n-1} cells.

As the plastic deformation of a cell of level n is stipulated by plastic deformations of its component cells of a level $(n+1)$, we suppose

$$e_p^n = \left\langle e_p^{n+1} \right\rangle, \tag{1}$$

where the angular brackets mean averaging by volume of n level cell.

We assume that the stress tensor and plastic deformation tensor of a cell of level n and its component 27 cells corresponding tensors of level $n+1$ are connected by a K r ö n e r–s tionship

$$\sigma^{n+1} - \sigma^n = M\left(e_p^n - e_p^{n+1}\right), \tag{2}$$

where M, in the common case, is a tensor of the 4^{th} rank. In the present work we substitute M by scalar magnitude. Below it is referred to as the parameter of accommodation. The sense of the title will be clarified during the discussion of the computer experiment outcomes.

The last relation shows that the difference between the plastic deformation of any cell of $(n+1)$ level and an average value of this strain in limits of the corresponding cell of the n level leads to the inner microstresses which seek to level these strains. That's why there happens the redistribution of stresses in limits of a cell of level n and the inhomogeneous SSS arises inside the complicated cells.

The relation (1) allows one to calculate plastic deformation of complicated cells through plastic deformation of their components. The plastic deformation of simple cells is determined by the mechanism of a strain operating in them.

In particular, for plastic deformation realized by means of a sliding of dislocations, the velocity of plastic deformation is calculated by toting components, stipulated by all systems of sliding operating in cell. In this case, for small elastic-plastic deformations the magnitude

$\dot{e}_p$ is calculated by the formula

$$\dot{e}_p = \frac{1}{2}\sum_{\alpha}\dot{\gamma}^{\alpha}\left(s^{\alpha}m^{\alpha} + m^{\alpha}s^{\alpha}\right), \tag{3}$$

where m^{α} and s^{α} are vectors of normal to the plane of sliding and vector of direction of sliding in system α; $\dot{\gamma}^{\alpha}$ – velocity of shear strain in system α.

The magnitude of $\dot{\gamma}^{\alpha}$ is determined by tangential stresses τ^{α} operating in system α. The magnitude of τ^{α} is calculated in a usual way by the tensor of stresses of the corresponding cell:

$$\tau^{\alpha} = m^{\alpha}s^{\alpha} : s^{\alpha}. \tag{4}$$

The relations connecting $\dot{\gamma}^{\alpha}$ with τ^{α} for various mechanisms controlling the dislocation migration can be found in a number of publications on physics of plastic deformation, in particular according to M.F.Ashby [8]

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0^{\alpha}\exp\left(-\frac{\Delta F}{kT}\left(1-\left(\frac{\tau^{\alpha}}{\tau_c^{\alpha}}\right)^{p}\right)^{q}\right), \tag{5}$$

where ΔF is the energy of activation necessary for overcoming of obstacles in a lack of external stresses; τ_c^{α} – critical tangential stress for system α; p and q – parameters depending on the mechanism controlling the dislocation migration ($0 \le p \le 1$, $1 \le q \le 2$); k – Boltsman constant; T – temperature; $\dot{\gamma}_0^{\alpha}$ – some parameter describing system α.

According to the cellular automata concept the process of SSS forming is researched in discrete time t_m with a step of discretization Δt ($t_m = m\Delta t$, where m is the integer value). At the upper level we set the dependence of operating stress on time $\sigma^1 = \sigma^1(t_m)$. At an initial moment of time ($m = 0$) we suppose that the plastic deformations e_p^n are equal 0 at all levels.

Relation (2) will be written in a modified form

$$\sigma^{n+1}(t_m) - \omega\sigma^n(t_m) = M\left(e_p^n(t_{m-1}) - e_p^{n+1}(t_{m-1})\right). \tag{6}$$

This allows us to calculate cell stresses at t_m by the plastic deformations in the previous instant t_{m-1}.

The relations (1)–(6) enable one to determine the SSS of polycrystal under the given program of the upper level loading.

If the program of the deformation of material at the upper level is set, that is the tensor of total strains $\mathbf{e}^1 = \mathbf{e}^1(t_m)$ is known, the magnitude of $\sigma^1(t_m)$ is determined under the law of Hooke

$$\sigma^1(t_m) = E : e_e^1(t_m) \tag{7}$$

in dependence on the elastic strain $e_e^1(t_m)$, where E is the elasticity modulus tensor.

Magnitude of elastic strain is calculated by the formula

$$e_e^1(t_m) = e^1(t_m) - e_p^1(t_{m-1}). \tag{8}$$

The relations (1)–(8) enable one to determine the SSS of polycrystal under the specific deformation program at the upper level.

3. Computer realization of the model

Basing upon the described above model of polycrystal deformation we have created a software package. During the creation of this package the object-oriented programming approach was used, where the cell of the cellular automata unit is an object of a programming language. In the given work as such language we used Delphi programming environment working under the control of Windows–95 operating system. It conveniently combined the object-oriented programming approach and visualized construction of programs both from standard and user-designed programming components.

The RAM volume is critical for work of the program. For instance, during simulation of 4-levels system with a possibility of only one sliding system in cells of the lower (4-th) level the program required about 5 Mb of RAM. In that case it was desirable to use a computer with more than 8 Mb of RAM, so that the Windows memory distribution system would allow program to use real RAM instead of swapping to the virtual memory (hard drive). Otherwise the execution speed of application will be low, that will not allow to carry out real-time numerical experiments. Program was executed on the Pentium–166 MMX computer with 32 Mb of RAM. Under such conditions the calculation of an average program of complex arbitrary loading of polycrystal takes about 3–5 minutes of computing time.

4. Outcomes of computer experiments

As an example we describe the results of experiments on simulation of complex deforming of α-Fe polycrystals. The parameters of formula (5) are taken from Ashby's book [8]: $\Delta F = 0.5\mu_0 b^3$ $b = 2.48 \cdot 10^{-10}$ – module of a Burgers vector; $\mu_0 = 6.4 \cdot 10^{10}$ Pa – shear modulus; $\tau_c = 1.7 \cdot 10^{-3} \cdot \mu_0$, $T = 293$ K.

In fig.2 the calculated curve of hardening according to the program of polycrystal deforming (tab. 1) is shown.

Table 1

Program of complex deforming

Step №	e_{xx}	e_{yy}	e_{zz}	e_{xy}	e_{yz}	e_{zx}
1	0	0	0	0	0	0
2	0.005	–0.005	0	0	0	0
3	0	0	0	0	0	0
4	0	0	0	0.005	0	0

Tab. 1 contains e_{ij} components of a complete strain tensor for material macrounit (cell of the 1st level). The following facts are interesting. At the unloading and loading in the opposite direction (step 3) the Baushinger's effect is observed. At the deforming by a shift on a step 4 the temporal unloading of a material happens, then the curve of hardening goes as a prolongation of a previous step curve. In such a way the known effect of a uniform curve of hardening is exhibited.

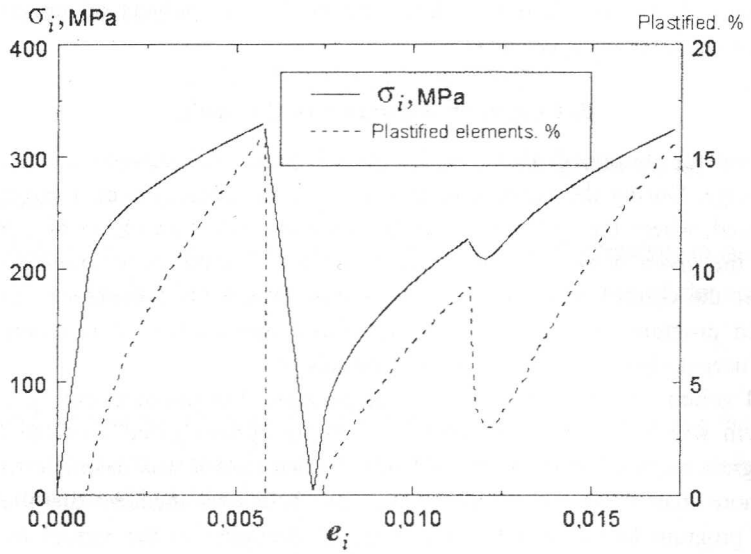

Fig. 2. Hardening curve and number of plastified elements at complex loading of α–Fe polycrystal.

In fig. 3 the outcomes of calculations of deformation in direction of the 2nd step of tab. 1 under the various values of parameter M of formula (2) are shown. According to this formula the physical sense of M is in the accounting of ability of the structural elements to accommodate to each other. The higher M, the less the ability to accommodation, i.e. there is a stronger reaction of the environment to a «stranger». From fig.3 it follows that the higher is the magnitude of M, the higher is a curve of hardening under the same remaining conditions of experiment.

Fig. 4 shows the influence of the number of acting sliding planes on the shape of material hardening curve. It is clearly seen that hardening curve lowers with the growth of the number of planes involved.

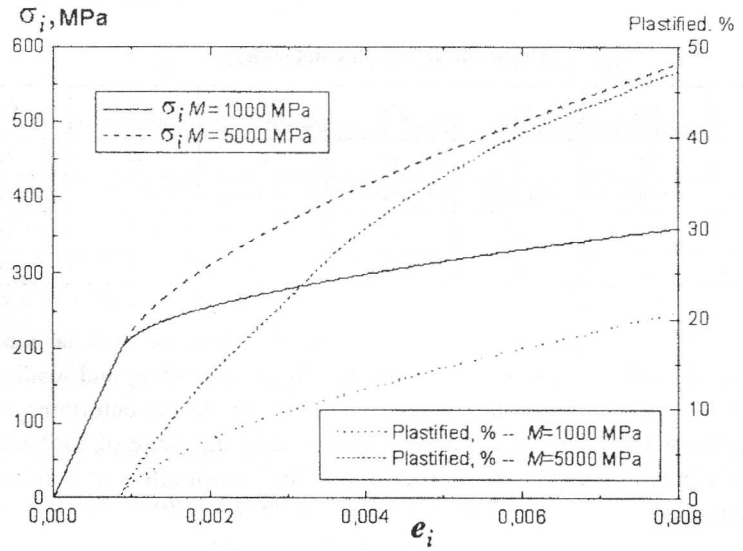

Fig. 3. Influence of accommodation factor M on the hardening curve and amount of plastified elements

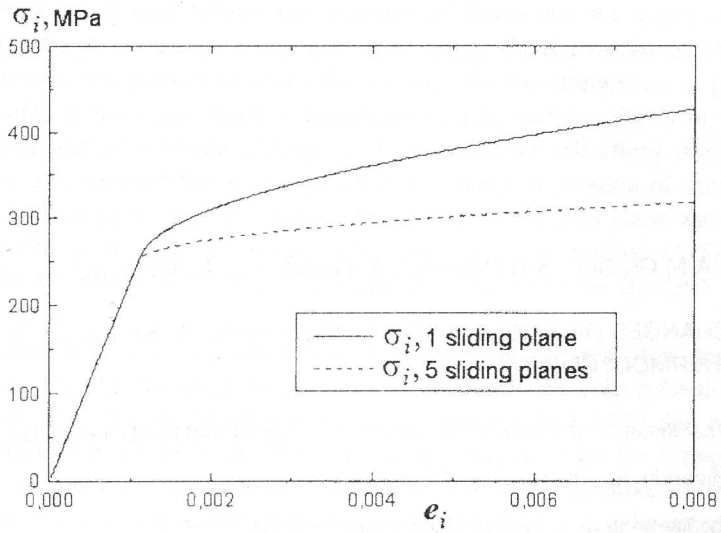

Fig.4. Influence of the number of acting sliding planes on hardening curve

5. Conclusion

The computer model of a strain of polycrystals based on the concept of cellular automata is developed. The model allows one to investigate polycrystal as a multilevel hierarchical system and to study singularities of this system behavior depending on a structure of material, strain mechanisms at the lower levels, program of loading and/or deformation at the upper level, temperature and other parameters. It allows one to connect in the uniform system the outcomes of research carried out at various scale levels, and to approach to the solution of a problem dealing with the prediction of properties of a material subjected to plastic deformation.

1. *Hill R., Rice J.R.* Constitutive Analysis of Elastic-Plastic Crystals at Arbitrary Strain. – J. Mech. Phys. Solids, 1972, **20**, p. 401–413.
2. *Asaro R.J.* Crystal plasticity. – Trans. ASME, Ser. E, J. Appl. Mech., 1983, **50**, No. 4b, p. 921–934.
3. *Mokhel' A.N., Salganik L.R., Khristianovitch S.A.* Plastic Deformation of Strengthened Metals and Alloys. Indicial Equations and Calculations. – Izvestiya of USSR Acad. Of Sc. Solid Body Mechanics, 1983, № 4, seconds 119–141.
4. *Toffoli T., Margolus N.* Cellular Automata Machines: Transl. to Rus. – Moscow, Mir publishers, 1991. – 280 pages.
5. *Preston K., Duff M.* Modern Cellular Automata, Theory and Applications, Plenum Press, 1994.
6. *Hornbogen E. Fine*, Coarse and Fractal Microstructures. – Prakt. Met, 1986, **23**, p. 258–267.
7. *Vladimirov V.I., Romanov A.E.* Disclinations in Crystals. – Leningrad, Nauka publishers, 1985. – 223 pages.
8. *Frost H.J., Ashby M.F.* Deformation – Mechanisms Maps. Pergamon Press, 1982.