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DYNAMIC RECRYSTALLIZATION OF TI-BASED MATERIALS AT CRACK SURFACES AT ELEVATED TEMPERATURES – HYBRID CELLULAR AUTOMATA SIMULATION

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Abstract. In the study a Hybrid discrete-continuum Cellular Automata approach (HCA) based on coupling classical thermomechanics and logics of CA-switching to simulate new phase generation and grain growth is proposed. On the basis of the HCA the numerical experiments on thermal-activated recrystallization of pure titanium in the vicinity of crack edges were conducted. In doing so the 3D cellular automaton simulates the behavior of the V-notched specimen region that imitates the crack tip vicinity. Numerical experiments are aimed at calculating heat expansion in the material under study through taking into account thermal stresses accumulation and microrotation initiation. The latter gives rise to generation of new defects and increasing the local entropy

1 INTRODUCTION

Over the last 50 years, the rapid development of aircraft and space technology as well as ever-increasing demands for equipment in the steel industry emerge new problems for the design of materials and structures operating under extreme conditions. Among them are materials employed for manufacturing nozzles for jet engines, tuyeres and crystallizers of

blast furnaces, etc. High temperature gradients and drops, powerful thermal impacts at engine start or filling melt into the crystallizer, etc., with the regard of cyclic repetition of the processes result in catastrophic degradation of the materials used. The material structure degradation is of very complex nature and is associated with various interdependent and simultaneously developing processes. The latter are accompanied by rearrangement of the internal structure of the substrate material, cracking and spallation of the protective coating, necleation of the brittle thermal-grown oxide layer, etc.

It is well known that experimental studies of materials under extreme condition and subsequent full-scale tests of semi-ready structures are very laborious and expensive. In this regard, theoretical predictions based on computer experiments are very relevant. Hard requirements for new materials call for the necessity to design and develop new advanced methods of computer simulation of the heterogeneous media behavior under extreme loading conditions.

The above said is of particular importance at the design of steam turbine blades. Steam turbines are used in various steam power plants (coal, nuclear, oil), combined cycle power plants as well as combined heat and power plants. Titanium alloys are popular as the blade materials in steam turbines, particularly in low pressure steam turbines that are considered to most significantly affect the power output, size and efficiency of steam turbines. The most promising ways of further increasing the efficiency of steam turbines is by extending the lengths of low pressure steam turbine blades and by increasing the steam reheat temperature. However, this results in substantial centrifugal stresses on blades and rotors and creep effects. As a consequence, advanced titanium alloys and manufacturing processes are needed to design the blades with sufficient reserve strength. Moreover, one of the most significant tasks is the coupled problem of cracking and the simultaneous recrystallization process under heat loading.

Recrystallization processes being applied to materials for steam turbines have been recently very successfully simulated [1, 2]. However, due to the intricate and complexity of the theoretical research of these processes, the development of new simulation methods seems to be very relevant.

In the current research the authors propose a Hybrid discrete-continuum Cellular Automata approach (HCA) based on coupling the classical thermomechanics and logics of CA-switching to simulate new phase generation and grain growth [3]. On the basis of the HCA the numerical experiments on thermal-activated recrystallization of pure titanium in the vicinity of crack edges were conducted. In doing so, the 3D cellular automaton simulates the behavior of the V-notched specimen region that imitates the crack tip vicinity. Numerical experiments are aimed at calculating heat expansion in the material under study through taking into account thermal stresses accumulation and microrotation initiation. The latter gives rise to generation of new defects and increasing the local entropy. Every “newly-nucleated” grain has zero dislocation density, so the gradient of the latter gives rise to additional driving force for the growth of new grains (along with thermal gradient).

The current study is aimed at continuation of our previous investigations already reported at the ECCOMAS-2016 congress. In the paper we concentrated on developing a new advanced and improved modeling algorithm. The latter ensures carrying out detailed studies of the processes related to rearrangement of the internal structure at the crack tip under intensive thermal loading. It should noticed that, the next stage of this study will be related to

finding out the model parameters being correspondent to physical characteristics of the specific material and comparison of the simulation results with experimental ones.

2 SIMULATION TECHNIQUE FOR RECRYSTALLIZATION AND GENERATION OF NEW PHASE ON THE BASIS OF CELLULAR AUTOMATA

This paper is devoted to development of the new algorithm for the grain structure recrystallization with taking into account the possibility of a twin-like growth of new phase crystallites. The discrete-continuum method of heat transfer was designed by the authors earlier [4, 5]. The transfer of mechanical energy within the framework of the hybrid approach of cellular automata was reported in [6-10]. The ideas of the modeling were inspired by the results reported in the book [11] as well as papers [12, 13]. Within the framework of the HCA method, the space occupied by the simulated specimen is represented as a cellular automaton, i.e. as a set of ordered active elements. In doing so, every element imitates an immovable region of space related to particular material being characterized by the following numerical parameters: heat capacity, thermal conductivity, density, etc. Additional material parameters used in model will be described below at explanation of the algorithm details. Note that the active element of the cellular automaton itself is stationary; however mass and energy flows to take place in it gives rise to changing of its properties in time.

In order to determine the temperature of the elements, a discrete model of heat transfer in a heterogeneous medium should be introduced [4, 5]. The values of the temperature, deformation, thermal conductivity, heat capacity and coefficient of linear thermal expansion of each element are specified as initial conditions. Then, for each n-th time step, a new value of the element's temperature is calculated taking into account the heat fluxes affecting from each neighboring element:

$$T_i^n = T_i^{n-1} + \frac{1}{c_i \rho_i V} \sum_{k=1}^{N} Q_{ik}^n , \tag{1}$$

where T_i^{n-1}, T_i^n – temperatures of i-th element at n-1-th и n-th time steps, c_i – heat capacity of i-th element, ρ_i – density of i-th element, V – element volume, Q_{ik}^n – the flow of thermal energy from a neighboring element with an index k into the element under consideration with index i at n-th time step, N – the number of neighbors. Hereinafter, all upper letter indices mean the step numbering in time, unless otherwise is specified. The change in thermal energy Q_{ik}^n is calculated on the basis of the Fourier law:

$$Q_{ik}^n = \frac{\lambda_{ik} \Omega}{l} \left(T_k^{n-1} - T_i^{n-1} \right) \Delta\tau . \tag{2}$$

Here λ_{ik} – coefficient of cross heat conduction, l – distance between the centers of the elements under consideration, Ω – area of adjacent face, $\Delta\tau$ – value of the time step.

As a result of inhomogeneous thermal expansion, internal thermal stresses are accumulated in various structural elements, which in turn are transformed into flows of mechanical energy being redistributed over the mesh of the cellular automaton. Within the framework of the method, grain boundaries were explicitly taken into account including with regard of their

curvature and misorientation angles of the crystal lattice. The developed algorithms have made possible to calculate the magnitude of the local force moments, the vorticity tensor and dissipation of torsion energy through forming new defect structures. There is no detailed consideration of the algorithm subtleties for modeling of the elastic energy transportation in this paper since it was widely described earlier in [6-10].

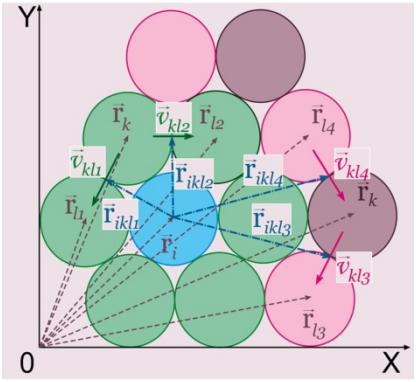


Figure1: A schematic for calculating the angular rate of material torsion for a cell automaton element

The angular velocity of the *i*-th element under the action of the matter flow through the boundary of the *k*-th and *l*-th elements (each *k*-th element is located at the 1st coordination sphere of the *i*-th, while each *l*-th – at the intersection of the 1-st coordination spheres of the *i*-th and the corresponding *k*-th elements) is calculated as follows (see Fig. 1):

$$\vec{\omega}_{ikl} = \frac{\vec{r}_{ikl} \times \vec{v}_{kl}}{\left|\vec{r}_{ikl}\right|^2}. \tag{3}$$

The matter flow velocity at the boundary of the *k*-th and *l*-th elements is calculated using the Thornbull relation:

$$\vec{v}_{kl} = m_{kl}(p_l - p_k)\vec{n}_{kl}, \tag{4}$$

where p_l, p_k – values of pressure (hydrostatic stress) in the *k*-th and *l*-th elements, $\vec{n}_{kl}$ - the vector of the normal to the boundary of the *k*-th and *l*-th elements, m_{kl} - the mobility of the boundary between the *k*-th and *l*-th elements.

The total angular velocity of the *i*-th element is defined as the following sum:

$$\vec{\omega}_i = \sum_{k=1}^{K}\sum_{l=1}^{L}\vec{\omega}_{ikl}. \tag{5}$$

Here K – the number of elements at the 1st coordination sphere of the *i*-th element, L – the number of elements at the intersection of the 1st coordination spheres of the *i*-th element and each *k*-th neighbor.

The three-dimensional rotation angle of the *i*-th element over the time $\tau(\Delta\vec{\gamma}_i)$ is proportional to the total angular velocity:

$$\Delta\vec{\gamma}_i = \vec{\omega}_i\tau. \tag{6}$$

The variation of the force moment of the *i*-th element over the time τ ($\Delta\vec{M}_i$) is calculated as follows:

$$\Delta\vec{M}_i = \frac{G\pi r_c^3 \Delta\vec{\gamma}_i}{2} = \frac{G\pi r_c^3 \vec{\omega}_i \tau}{2}. \tag{7}$$

Here G – the shear modulus of the material being contained in the *i*-th element, r_c – the radius of the element. The term being responsible for the accumulation of latent energy of defects is written as follows:

$$\left[\Delta\vec{A}_d\right]_i^n = \frac{k_{tors} G_i \left|\Delta\vec{\gamma}_i^n\right| \pi r_c^3}{2} \Delta\vec{\gamma}_i^n. \tag{8}$$

Here $\boldsymbol{k_{tors}}$ – defect accumulation rate (can be measured experimentally).

Note that the expression (8) possesses very general nature and, depending on the constructed switching rules of the cellular automaton can bring the meaning of the energy necessary to run a reversible structural-phase transformation. Then the coefficient $\boldsymbol{k_{tors}}$ can be calculated on the basis of the atomic configurations of the initial and final states.

At the first stage of the recrystallization simulation a specimen is modeled by a cellular automaton network of L active elements. The network is divided in M clusters, which are representing single grains of the material. Each *i*-th element has initial values of the temperature T_i^0, thermal energy Q_i^0, elastic energy E_i^0 and dislocation energy Θ_i^0. Each *I*-th grain is also characterized by Euler orientation angles ψ_I, φ_I, η_I. The following algorithm is proposed for the simulation of the generation and growth of new phase nuclei under thermal loading. For each element with index *i* the probability of a new grain nucleus generation inside the *I*-th grain of initial phase ($(p_{sw})_i^n$) is based on the temperature of the element T_i^n which is calculated at every time loop of the algorithm. When the temperature of certain elements reaches the critical value T_{sw1}, its probability takes a non-zero value according to the equation:

$$(p_{sw})_i^n = \begin{cases} 0, & T_i^n < T_{sw1}; \\ 2(p_{sw})_{\max} \dfrac{T_i^n - T_{sw1}}{T_{sw2} - T_{sw1}}, & T_{sw1} \le T_i^n < (T_{sw1} + T_{sw2})/2; \\ 2(p_{sw})_{\max} \dfrac{T_{sw2} - T_i^n}{T_{sw2} - T_{sw1}}, & (T_{sw1} + T_{sw2})/2 \le T_i^n < T_{sw2}; \\ 0, & T_{sw2} \le T_i^n. \end{cases} \tag{9}$$

In this case, T_{sw2} is the temperature threshold at which the probability of nucleating a new phase grain becomes equal to zero. If the element under consideration becomes a nucleation center of a new grain then all adjacent elements located at the first coordination sphere automatically join it. Thus, the grain nucleus of the new phase represents a group of elements.

The nucleation of a new grain entails a reduction of the defects density down to a minimum value for all the elements that have joined it. If this takes place the variable L being responsible for the total number of grains in the specimen is increased by 1, while the index of the new grain becomes equal to L. When all the elements of the cellular automaton have been

analyzed the growth of new grains is realized within the framework of the recrystallization algorithm being introduced by the action of the defect density gradients, thermal and elastic energy. The following calculations are performed at each *n*-th time step of the algorithm. The K_i^n parameter that is equal to the number of neighbors belonging to grains with orientation angles different from θ_I (orientation angle of the *I*-th grain containing the *i*-th element) by less than θ_{HAGB} is calculated for each *i*-th element. The probabilities of transition of *i*-th element from the current *l*-th grain in each of the grains (with the index *K*) is computed:

$$P_{ik}^n = P_{ik}^n (E_K^{n-1} - E_I^{n-1}),\ 1 \le k \le K_i^n. \tag{10}$$

First of all, the specific energy g_{IK} of the boundary between grains *I* and *K* is calculated by the following relation [11]:

$$\gamma_{IK} = \gamma_{HAGB} \frac{\theta_{IK}}{\theta_{HAGB}} \left(1 - \ln \frac{\theta_{IK}}{\theta_{HAGB}}\right), \tag{11}$$

where $\theta_{IK} = |\psi_I - \psi_K|$ - grain misorientation angle of *I*-th and *K*-th grains.

Further, according to the Turnbull equation, the grain boundary velocity is calculated:

$$v_{ik}^n = (m_{ik}^n p_{ik}^n + \hat{m}_{ik}^n \hat{p}_{ik}^n + \tilde{m}_{ik}^n \tilde{p}_{ik}^n) e^{-\frac{2\Omega\gamma_{IK}}{k_B (T_i^{n-1} + T_k^{n-1})}}, \tag{12}$$

where

$$p_{ik}^n = \frac{Q_i^{n-1} - Q_k^{n-1}}{V}, \tag{12a}$$

$$\hat{p}_{ik}^n = \frac{E_i^{n-1} - E_k^{n-1}}{V}, \tag{12b}$$

$$\tilde{p}_{ik}^n = \frac{\Theta_i^{n-1} - \Theta_k^{n-1}}{V}. \tag{12c}$$

These are the driving forces, initiated by the gradients of thermal energy, elastic energy and defect energy, correspondingly. Here m_{ik}^n - grain boundary mobility in thermal recrystallization process, $\hat{m}_{ik}^n$ - grain boundary mobility in mechanical ("cold") recrystallization process, $\tilde{m}_{ik}^n$ - grain boundary mobility in recrystallization process initiated by dislocation density gradient, Ω – area of adjacent active elements, k_B – Boltzmann's coefficient , V – the volume of single active element.

The energy of defects in *i*-th element Θ_i^n at *n*-th time loop is calculated by the following relation:

$$\Theta_i^n = -d_i \rho_i^n G_i b_i^2, \tag{13}$$

where d_i is the coefficient depending on the spatial distribution of the defects, ρ_i^n is the density of defects, G_i is shear modulus, b_i is the Burgers' vector.

When calculating the probability of the grain growth the anisotropy should be taken into account in order to allow for the specific features of the simulated processes. The former is related to the translational symmetry of the crystal which is determined by the crystalline lattice type and orientation, i.e. by directions and relative lengths of its basis vectors $\vec{a},\vec{b},\vec{c}$. The maximum relative length of the basis vector is equal to unit.

Thus, the value of the grain boundary velocity v_{ik}^n must be corrected through taking into account the relative location of the expected grain growth vector ($\vec{u}$) as well as $\vec{a},\vec{b},\vec{c}$ ones.

i) The cosine moduli of the angles between the vector $\vec{u}$ and each of the $\vec{a},\vec{b},\vec{c}$ ones are computed:

$$\begin{aligned} \alpha &= |\cos(\vec{u},\vec{a})|, \\ \beta &= |\cos(\vec{u},\vec{b})|, \\ \gamma &= |\cos(\vec{u},\vec{c})|. \end{aligned} \tag{14}$$

ii) Among the vectors $\vec{a},\vec{b},\vec{c}$, the one is chosen whose cosine with the vector $\vec{u}$ has the maximal modulus:

$$\delta = \max(\alpha,\beta,\gamma) = |\cos(\vec{u},\vec{d})|. \tag{15}$$

iii) By taking into account the anisotropy effect coefficient *k*, the value v_{ik}^n is redefined:

$$\widetilde{v}_{ik}^n = |\vec{d}\,|\, v_{ik}^n\, e^{k\cdot(\delta-1)}, \tag{16}$$

here $k >= 0$ (if $k = 0$, then the lattice anisotropy is absent). It should be stressed, that when the lattice anisotropy s absent, as well as when the vector $\vec{u}$ is co-directed with one of the lattice vectors, the grain boundary movement rate reaches its maximum value.

The switching probability P_{ik}^n of the active element is calculated by the following formula:

$$P_{ik}^n = \frac{\max(0,-v_{ik}^n)\cdot\tau}{l}, \tag{17}$$

where τ is the value of the time step. According to these probabilities, the switches of active elements occur.

When some *i*-th active element reached the necessary "level of switching", the index of state (grain index) should be found, which will become a new state of the element. Here the "level of switching" depends on the variation between the probability P_{ik}^n and random number that generated each time loop for each element.

Along with the grain that will "catch" the element, the index of neighboring active element belonging to the "catching" grain should be calculated. For this purpose one can construct some kind of membership function, which accounts for all switching probabilities P_{ik}^n:

$$f_i^n(\eta,k)=\frac{1}{2}-\frac{\left(\eta-\sum_{j=1}^{k-1}P_{ij}^n\right)\left(\eta-\sum_{j=1}^{k}P_{ij}^n\right)}{2\left|\eta-\sum_{j=1}^{k-1}P_{ij}^n\right|\left|\eta-\sum_{j=1}^{k}P_{ij}^n\right|}. \tag{18}$$

This function is equal to 1 when the random number η belongs to the interval

$$\left(\sum_{j=0}^{k-1}P_{ij}^n;\sum_{j=0}^{k}P_{ij}^n\right), \tag{18a}$$

and it is equal to zero when η is beyond the interval (10a). Moreover, when the element stays in the old grain,

$$k=K_i^n+1 \tag{18b}$$

and

$$P_{i,K_i^n+1}^n=1-\sum_{j=1}^{K_i^n}P_{ij}^n\cdot \tag{18c}$$

Summing up the aforesaid reasoning, the new state (grain index) of *i*-th element at the next time loop will be as follows:

$$Z^{n+1}=\sum_{k=1}^{K_i^n+1}k\cdot f_i^n(\eta,k)\cdot \tag{19}$$

The relation (8) makes it possible to calculate the part of the microflows energy of the material in the cell automaton element, which comes to the formation of deformation defects. From the thermodynamics point of view this means a local variation of the entropy and temperature:

$$\left[\Delta E_d\right]_i^n=T_i^{n-1}\Delta S_i^n+S_i^{n-1}\Delta T_i^n. \tag{20}$$

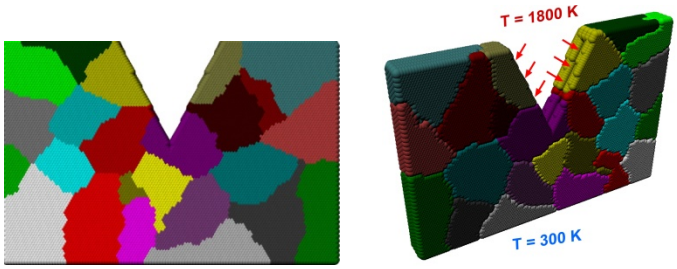
These relationships will be further used for the criteria of twin structures nucleation as well as subsequent failure of the material.

3 NUMERICAL EXPERIMENTS ON RECRYSTALLIZATION

On the basis of the Hybrid Cellular Automata approach numerical experiments for thermal-activated recrystallization of pure titanium near the crack edges were conducted. The 3D cellular automaton simulates the V-notched specimen region which imitates the vicinity of the crack. In this numerical experiment heat expansion in the material was taken into account along with thermal stresses accumulation and microrotation initiation. The latter gives rise to new defects generation and local entropy increase. As was mentioned above, every "newly-nucleated" grain has zero dislocation density. In doing so the dislocation density gradient initiates additional driving force of new grains growth (along with thermal gradient).

The specimen was simulated by the cellular automata with FCC (Face Centered Cubic) type packing of elements with characteristic size of 1 μm. The specimen dimensions were

$80 \times 120 \times 10$ μm^3. The initial temperature of each element was set at 300 K, the initial values of strains and stresses were equal to zero. The time step was set at 1 ns. For numerical calculation the material constants were taken being typical for pure Ti. In all the numerical experiments the inner surface of the notch was heated at temperature of 1800 K. The scheme of the numerical experiment is depicted in Fig. 2.



a) b)

Figure 2: Initial structure of the specimen simulated (a) and the loading scheme (b)

The figures below depict the evolution of the spatial distribution of the temperature, grain structure, elastic energy, local force moments and defect accumulation rate.

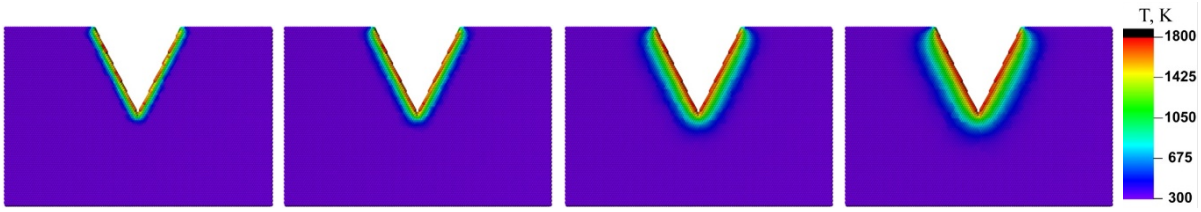


Figure 3: Evolution of the temperature field during heat loading in the vicinity of the notch tip

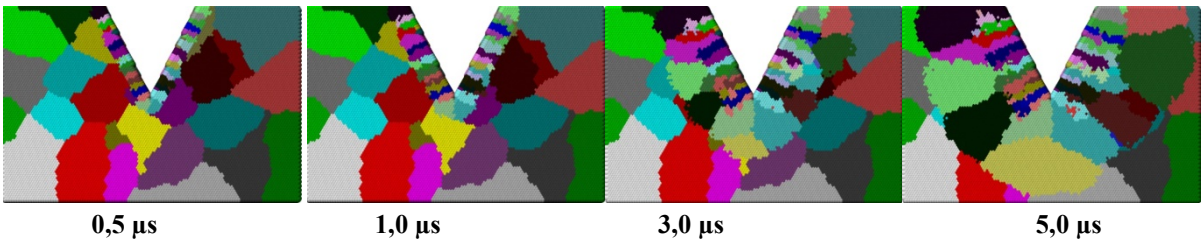


Figure 4: The patterns of grain structure at various time steps

As one can see from all the grain structure distribution patterns, a high temperature gradient gives rise to a characteristic columnar-like growth of the grain structure. The latter is directed from the region with elevated temperatures towards the cooler bulk material. Along with the nucleation and the columnar-like growth of new grains within the bulk material the growth of old ones takes place. In the framework of the current approach, the thermal expansion of the material that initiates the occurrence of thermal stresses is simulated. The inhomogeneous field of thermal stresses generates the appearance of local force moments that are the source of the crystal lattice curvature. Further, the lattice curvature is relaxed at

microrotations giving rise to the increasing defect density in the material. A detailed algorithm and simulation results of these processes are presented in [4]. Since this study is not focused on the analysis of mechanical field effect, the below described results are rather illustrative and mostly give the ideas of further development of the algorithm. It should be particularly noticed that the value of thermal stresses is estimated through the ratio of the elastic energy over the volume of the local structural element. Figure 5 illustrates the thermal stress development in the surface layer.

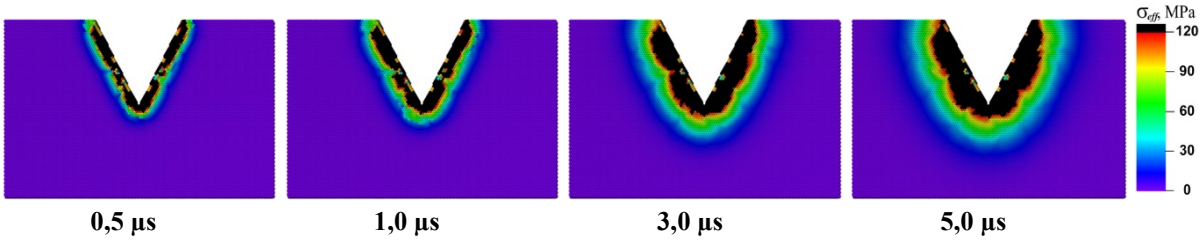


Figure 5: The evolution of the specific elastic energy at the specimen surface at various time steps

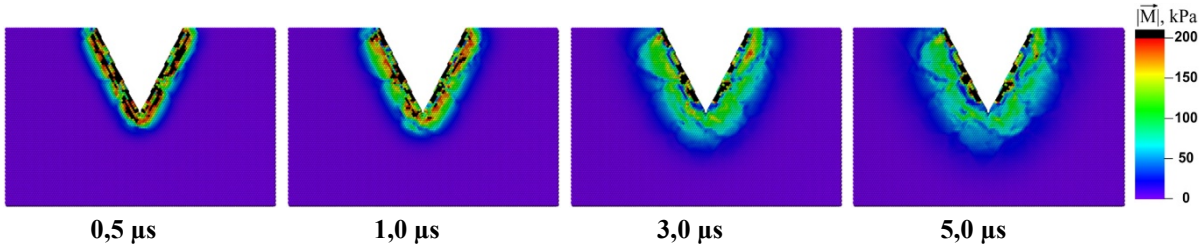


Figure 6: The spatial distribution of the specific force moments at the specimen surface

In this regard, the pattern of spatial distribution of the local force moments in the bulk specimen (Fig. 7) and its surface layer (Fig. 6) are of particular informativeness. The figures illustrate the distribution of the specific values of the local force moment being expressed in Pascals. Despite the fact that these values are three orders of magnitude lower than the level of effective stresses, it is quite enough to generate a substantial curvature of the crystalline lattice and disrupt its translational symmetry.

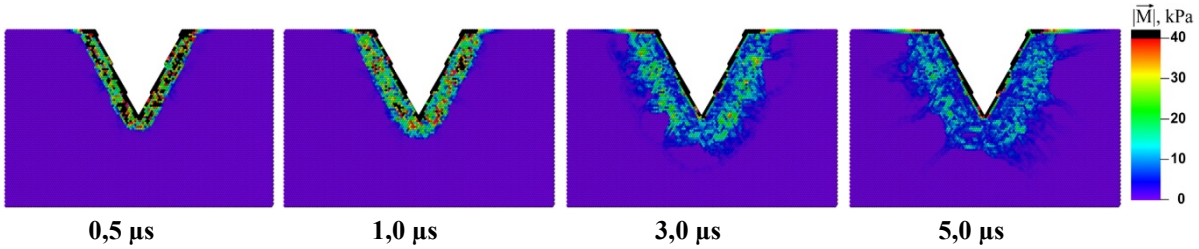


Figure 7: The spatial distribution of the specific force moments in the bulk specimen at various time steps

The spatial distribution of the ratio of the torsion energy increment over the elastic energy influx per the computational algorithm step is presented in Fig. 8. This parameter is directly related to the rate of new defective structures generation in the material.

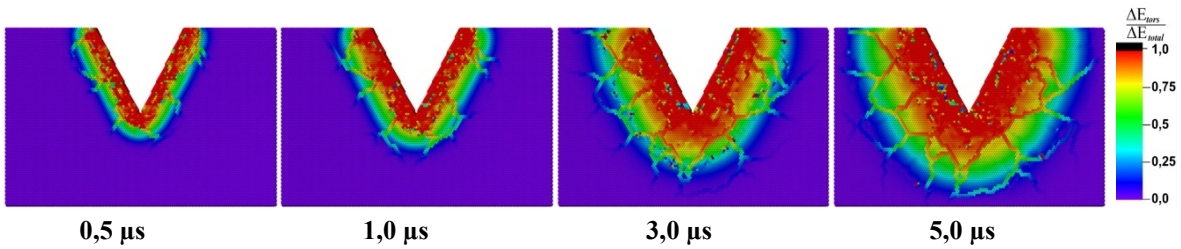


Figure 8: The evolution of the defect accumulation rate in the specimen surface layer

4 CONCLUSIONS

- The new approach of Cellular Automata for the grain structure recrystallization simulation was developed with taking into account the possibility of a twin-like growth of new phase crystallites. The method combines CA-switching mechanisms for structure transformation simulation, classical thermal transfer and such mechanical effects, as thermal expansion and defect generation.
- It was shown that the material adjacent to the crack sides undergoes the changing of its crystal structure. The new grains are generated at the crack sides and grow to form column-like patterns to replace the initial grain structure. This fact results in significant local variation of all mechanical properties of the material. This study is a starting point for developing the algorithms to simulate deformation behavior of turbine blades containing fatigue cracks.
- It is shown that in the mostly heated regions of the specimen not only the nucleation of the new crystalline structure occurs, but the fraction of the elastic torsion energy increase is also very high. Under such conditions, the probability of twin structure nucleation is very high due to the deformation development by the torsion mechanism. The development twinning models will be the matter of the studies in the series of upcoming works.

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