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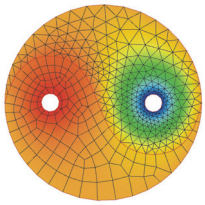

MICRO- VERSUS MACRO- MODELLING OF CREEP DAMAGE

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Abstract

In the present paper the continuous approach to model brittle-ductile transition in creep failure phenomenon is replaced by Cellular Automata (CA) model. This allows to back-up this complex phenomenon by relating it to microstructural changes.

In previous author's work the technique of CA has been developed for polycrystalline material structure modelling and brittle failure initiation. The same methodology is used in the present paper, where both ductile and brittle processes are of equal importance. The Hoff theory of ductile failure is implemented in Abaqus package and coupled with CA model of brittle failure. Thus, the proposed description falls into category of Cellular Automata Finite Element (CAFE) methodology applied successfully in metallurgy.

Concurrent running of both models yields effectively transition points on log-log diagram of time to failure. The results of above descriptions are compared with experimental observations reported in literature.

Key words: Cellular Automata, creep fracture, damage mechanics, CAFE

1. INTRODUCTION

Microscopic observations show that creep damage of metals at elevated temperature is affected heavily by material microstructure. For high loads and lower temperatures final failure is of ductile character, i.e. occurs mostly within material grains. In opposite case (low load and high temperature) inter-granular defects prevail causing brittle failure. For macroscopically observed transition region both micro-mechanisms come to interplay. Whereas the ductile failure can be well described by methods of continuum mechanics, the process of brittle deterioration exhibits more scatter as it is mostly governed by microstructure of grain boundaries.

The results of creep damage tests in constant temperature for polycrystalline materials can be approximated by two straight lines on time to failure versus strain rate log-log graph. The steeper line at longer times to failure and lower strain rates is connected with brittle failure. The second line of reduced slope for short times and large strain rates represents ductile damage. The region of both types of failure can be considered at macroscopic and microscopic levels, as well.

2. FAILURE IN CREEP CONDITIONS

2.1. Macroscopic description

It is well known that process of failure of polycrystalline materials in elevated temperatures is connected with deformation. This is reflected by the Monkman-Grant rule [12]:

$$\dot{\varepsilon}_s^{\beta} t_f = C \tag{1}$$

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where $\dot{\varepsilon}_s$ is steady state creep rate, t_f is time to failure, β, C are material constants. In most cases the value of parameter β is close to 1, so the Monkman-Grant relation can be written as

$$\dot{\varepsilon}_s t_f = C_{MG} \tag{2}$$

here the constant C_{MG}, called the Monkman-Grant constant, is strictly connected with strain to failure. The relation of strain to failure to the Monkman-Grant constant is called damage tolerance parameter and can be used to recognise damage mechanism [1]. The equation (2) was induced already in 1953 by Hoff [7] on the basis of theoretical considerations. He assumed that a bar of material, which complies with Norton creep law and under constant tensile load, fails due to loss of cross-section. The time to failure can be expressed as:

$$t_f = \frac{1}{Bn\sigma_0^n} = \frac{1}{n\dot{\varepsilon}_s} \tag{3}$$

where B, n are constants of Norton creep law, σ_0 is nominal stress. The Monkman-Grant constant for this case is equal to $1/n$. This is the upper limit of Monkman-Grant constant and indicates that the failure is caused by deformation [14]. It is therefore called ductile failure. Using the same equations Hoff also calculated a shape of the neck. He assumed that the material properties are homogenous but the cross section area is only slightly narrowed in the middle of the specimen. In such circumstances the time to failure can be calculated not only for constant load but also for constant true stress. The instability of creep deformation which is inherent with this description, is connected with value of creep index n, and the equation (3) is valid for $n>1$.

Obviously, Hoff assumptions do not allow calculating the true strain to failure that goes to infinity as cross section area goes to zero.

2.2. Continuum Damage Mechanics description

When the value of exponent β in equation (1) is less than 1 it means that the process of failure is developing faster that deformation process. In such a case the brittle failure occurs. It is connected with development of internal cavities (or cracks). The process can be described by Kachanov equation of damage development [8]. The time to failure calculated upon it can be expressed as:

$$t_f = \frac{1}{(m+1)A\sigma_0^m} = \frac{1}{(m+1)(A/B)\dot{\varepsilon}_s^{m/n}} \tag{4}$$

where m, A are material constants in Kachanov equation. Comparison of the equations (4) and (1) shows that the value of exponent β is equal to m/n. The equation (4) is derived from Kachanov damage evolution law under assumption that the stress is constant. When the test is made in constant load condition the cross area is decreasing and stress is increasing. This situation can be described by applying true stress concept to the Kachanov equation that yields time to failure in so called mixed mode:

$$t_f = \frac{1}{nB}\left[\frac{1}{\sigma_0^n} - \left(\frac{1}{\sigma_0^{n-m}} - \frac{B}{A}\frac{n-m}{m+1}\right)^{\frac{n}{n-m}}\right]. \tag{5}$$

This equation is valid only for nominal stresses less than characteristic value $\hat{\sigma}_0$ given by:

$$\hat{\sigma}_0 = \left(\frac{m+1}{n-m}\frac{A}{B}\right)^{\frac{1}{n-m}}. \tag{6}$$

When the nominal stress is greater than the value $\hat{\sigma}_0$ the ductile failure (equation (3)) prevails and the cross-section area of a bar under trension becomes zero faster than internal damage reaches its limit value. According to Kachanov theory strain to failure can be calculated from Norton equation and is of finite order. For small nomial stresses the reduction of cross section (at constant load) is small and there is no tertiary creep – damage tolerance paramter is close to one (according to this model). For larger nominal stresses (but still smaller than $\hat{\sigma}_0$) the reduction of cross section is noticable and the strain to failure is large but finite. The tertiary creep is modeled in this case and the damage tolerance parameter is larger than one. When the stresses are larger than $\hat{\sigma}_0$ solely the Hoff model is applicable and according to it the strain to failure and damage tolerance parameter tend to infinity.

2.3. Internal damage model

Another model is needed to obtain finite value of strain to failure in ductile case. Additional mechanisms have to be introduced like influence of internal voids. Such a model was proposed by Cocks and Ashby [3]. They showed that internal voids grow due to deformation of surrounding material and

cause the failure in the same time as obtained by Hoff at constant load. To calculate the strain at failure they assumed a criterion that area fraction of voids is equal to 0.25. This leads to the following formula:

$$\varepsilon_f \geq \dot{\varepsilon}_s t_f + 0.2\frac{l}{d} \tag{7}$$

where ε_f is strain to failure, $2l$ is the voids spacing and d is grain size. The second term in equation (7) is strain due to tertiary creep and is caused by the volume of voids at failure. This criterion of failure is connected with internal necking mechanism. It occurs when the size of voids is equal to spacing between them [5] and for spherical voids it gives the critical value of area fraction 0.25.

The values of strain to failure predicted by this model are larger than experimental ones [4]. This is because that the mean values of many parameters of the model are used, whereas the failure happens in the weakest section of specimen.

3. CELLULAR AUTOMATA FINITE ELEMENT APPLICATION

It was shown by Cocks and Ashby that the time to ductile failure for constant load test is the same irrespective if it is caused by reduction of external section or due to growth of internal voids. As the Kachanov model of brittle failure is a phenomenological one, it does not explain why the failure occurs.

The purpose of this paper is to replace the Kachanov differential equation formulated in terms of continuum mechanics, by the simulation of physical mechanisms of brittle failure. Cellular Automata (CA) are chosen as a tool suitable for this modelling. They were successfully used in modelling of plastic (time independent) failure [11,15] as they can deal with discontinuous and heterogeneous microstructure.

In a mixed mode failure two kinds of deterioration participate in damage development. They are of different scales, so models in different scales are needed. The ductile failure is modelled by Finite Element Model (FEM) implemented in Abaqus and the brittle failure by CA run at Gauss points of FE mesh. The FE model uses the Norton law to calculate the strains in creep condition and these strains are imposed as a loading of CA network.

3.1. FE model

In unidirectional tension under constant load, which is considered here, the states of strains and stresses are homogenous at macroscopic level. As Cellular Automata model is developed for plane strain state the corresponding plane strain elements CPE4I are used. The user subroutine UMAT is used for modelling the creep behaviour and for implementing Cellular Automata. The creep strains at macroscopic level are calculated according to the equation:

$$\frac{\partial \varepsilon_{ij}}{\partial t} = D^{-1}_{ijkl}\frac{\partial \sigma_{kl}}{\partial t} + B\sigma^{n}_{eff}\frac{\partial \sigma_{eff}}{\partial \sigma_{ij}} \tag{8}$$

where ε_{ij} is strain tensor, σ_{ij} is stress tensor, σ_{eff} is Huber-Mises effective stress, t is time, D_{ijkl} is elastic constants matrix, B, n are creep material constants.

The "damage zone" is modelled by 4 elements. There are 4 Gauss points in each element so 16 different CA have to be run in parallel. The remaining volume of the specimen can be described by elements without damage taken into account.

3.2. CA model of damage

The process of brittle failure is modelled with Cellular Automata. Brittle failure is strictly connected with development of intergranular voids. The voids nucleate at grain boundaries, and then they grow due to deformation or diffusion to coalesce forming a macroscopic crack.

The Cellular Automata represent the behaviour of Representative Volume Element (RVE) of the structure. The size of it must be chosen very carefully to maintain dimension relations in a real material. The parameters describing these relations are initial number of cells along RVE side N_{init} and number of grains in RVE n_{seed}.

One CA cell represents some piece of material (called mass cell) or a void (called empty cell). Every mass cell belongs to a grain, so the grain boundaries can be distinguished. The 2-D mesh is considered.

The first task is to model the initial microstructure of polycrystalline material. The picture of real microstructure or its substitutive image can be use for that purpose (see e.g. [9]). In this paper the discrete Voronoi tessellation described in previous papers [2,13] is applied. The initial vacancy concentration is modelled by some empty cells distributed randomly over RVE. The number of initial empty cells is calculated on the basis of assumed value of g_{dam0} parameter.

The second task is to spread the deformation over CA mesh. The deformation is calculated in every step by FE program. If this deformation is noticeable by CA mesh the deformation step is performed. The deformation is noticeable if the strain change is of order $2/N$, when N is actual size of RVE. The deformation procedure is based on Matic-Geltmacher model [11] adapted to grain structure in [2,13].

New mechanism is introduced to maintain the number of mass cells. Instead mass cells the number of empty cells is under control. This assumption makes the model more stable as the modelled process depends mainly on the number of empty cells. In previous models (e.g. [2]) this number was changing rapidly after deformation step. The number of mass cell is large (it is comparable with number of all cells) and small variations of it can be neglected.

After each deformation step some new empty cells are generated inside RVE, they correspond to vacancies generated by deformation [14], so the overall density is reduced.

The third task is to model the process of void growth. Generally speaking it can be caused by deformation or by diffusion. The deformation growth is modelled in deformation step. For brittle damage more important is diffusive growth. It results from grain boundary diffusion that dominates over the volume diffusion. The grain boundaries are vacancy sources providing "material" for voids nucleation and growth. The third kind of diffusion – surface diffusion is responsible for void shape. When it is slower than boundary diffusion the voids grow into cracks, when it is faster the void are more oval.

The diffusion step is performed in each automaton time step. The diffusion coefficient yields the time scale for the model according to the equation:

$$D = p\frac{\Delta l^2}{\Delta t} \tag{9}$$

where D is diffusion coefficient, Δl is the linear size of cell, Δt is time of one time step, p is the probability of state exchange with neighbouring cell. The diffusion is modelled using 2x2 blocks of cells using so called Margolus neighbourhood [10]. The number of empty cells is constant inside the block, but their position can change in random manner. In the next step the position of blocks is shifted by one cell so that the empty cells can move in any direction preserving the number of empty cells for whole RVE. The diffusion is possible only when energy of new configuration is equal or less to actual one. The energy is calculated as the sum of grain boundary energy and free surface energy:

$$J = w_{e-m}l_{e-m} + w_{g-g}l_{g-g} \tag{10}$$

where $w_{e\text{-}m}$ is weight factor for empty-mass border and $l_{e\text{-}m}$ is number of neighbouring pairs empty-mass cells within enlarged block, and $w_{g\text{-}g}$ is weight factor for grain-grain border and $l_{g\text{-}g}$ is number of neighbouring pairs belonging to different grains. The calculations are made within the block enlarged by one cell in each direction to ensure more stability of the system.

There is no special model for voids coalescence. They simply join with neighbouring voids forming larger void or crack. But when the spacing between neighbouring voids is small they do not grow independently as concentration of empty cells is less then at single void and the process of void growth is inhibited.

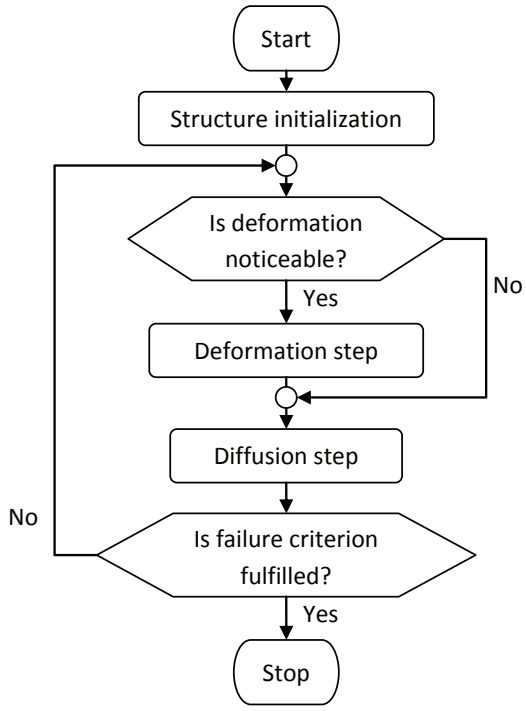

Fig. 1. *The flow chart of main CA steps.*

The RVE is assumed to be failed when the empty cells forms a crack spanning opposite sides of it. Additionally the damage parameter is calculated in every step as a linear projection of the greatest crack (connected area of empty cells) onto RVE side related to total RVE size. This parameter reaches value of one in a case of failure.

The summary of the CA algorithm is shown in figure 1.

4. EXAMPLE

The results of simulation of failure process in a bar under uniaxial tension are compared with experiment described by Feltham and Meakin [6]. They examined cooper bars in temperature of 723K in range of nominal stresses from about 15 MPa to 80 MPa. The material was oxygen free high conductivity (OFHC) copper of purity 99.99%, with grain mean diameter 30 μm. The results of experiment, presented in figure 2 allowed to calculate the parameters of Norton equation n=4.17, B=1.18E-12 $(\text{MPa})^{-n}\,\text{s}^{-1}$. The experimental points fit very well to Monkman-Grant rule giving the value of constants β=0.914 and C=0.162. Since β is close to one, the mechanism of failure can be attributed to the deformation. But when points for low stresses (below 30 MPa) are excluded from evaluation of the exponent β it becomes even closer to one (0.992). This suggests that these points indicate another mechanism of failure. The Monkman-Grant constant obtained for stress greater that 30 MPa is C_{MG} = 0.089 (according to [6] for wider range of temperatures the Monkman-Grant constant is equal to 0.055). It is much lower than $1/n$=0.24 so the mechanism of failure is connected with deformation but not solely with loss of cross-section like assumed by the Hoff theory.

Parameters of Kachanov equation were calculated from points below 40 MPa: A=5.04E-10 $(\text{MPa})^{-m}\,\text{s}^{-1}$, m=2.87.

4.1. CA parameters

The procedure of finding the proper values of CA parameters is based on real values of microstructure parameters. The CA parameters have to be limited to ensure efficiency of calculations. The main criterion for evaluating these parameters is fitting the final results of modelling to results of experimental macroscopic observations.

One of the important material parameters is the size of minimal diameter of cavities, but there is a big scatter of observed diameters. Theoretically it is from 0.2 μm to 0.05 μm [14] depending on stresses applied in the experiment. The size of smallest void is assumed to be 0.2 μm, thus it is the physical dimension of automaton cell. The grain diameter is about 150 cells, so the initial size of RVE should be $150\sqrt{n_{seed}} = 335$ cells for n_{seed}=5. The number of 321 was admitted for simplification. The higher number of grains, which corresponds to greater RVE (in physical units), requires higher number of cells.

Time step of automata is 10 s. It gives the diffusion coefficient for automata D=2.28E-16m^2s^{-1} (for p=1/6 in equation (9)). Comparing it with grain boundary diffusion coefficient for copper in test temperature δD_{gb}=153E-24m^3s^{-1} [14], the characteristic dimension for automaton of modelled diffusion can be calculated: $\frac{\delta D_{gb}}{D} = 0.211\mu\text{m}$. It is comparable to magnitude of cell size.

Initial density of empty cells is assumed to be 0.005. Coefficient of relative increase of empty cells per one deformation step is set to 0.1.

The weight factors for diffusion energy criterion was $w_{e\text{-}m}$=0 and $w_{g\text{-}g}$=1 to promote development of crack-like voids characteristic for brittle failure.

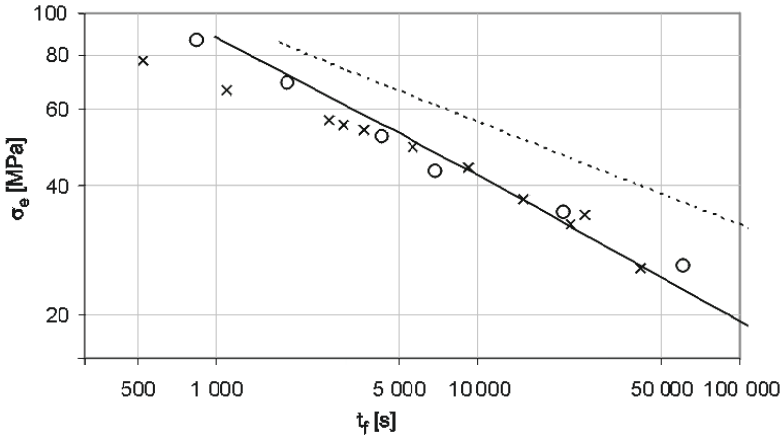

*Fig. 2. The relation between nominal effective stress σ_e and time to failure t_f. Results of experiment [6] are denoted by **x**, results of CAFE simulation by **o**, dashed line is for time to failure according to Hoff, solid line for mixed-mode Kachanov-Hoff theory.*

4.2. Results

Results of simulations are presented in table 1 and plotted in figure 2. The examined stress range was wider than that corresponding to mixed mode failure to verify passing to limit cases of brittle and ductile modes.

Times to failure obtained by simulations are in good correlation with experimental one for nominal stress range 30-60 MPa, for higher stress the values are too high but they are close to values calculated according Kachanov-Hoff theory of mixed-mode failure (equation (5)). The times to failure obtained by CAFE for stress below 30 MPa are too large. It suggests that influence of modelled diffusion is too weak to properly model the brittle failure.

Table 1. *Results of CAFE simulation.*

nominal stress	steady state creep rate	time to failure	strain to failure	Monkman-Grant constant	damage tolerance parameter
σ_0	$d\varepsilon_s/dt$	t_f	ε_f	C_{MG}	λ
[MPa]	[s^{-1}]	[s]	[%]	[%]	[-]
15	4.52E-08	7.21E+05	3.5	3.3	1.08
20	1.50E-07	1.90E+05	3.1	2.9	1.07
30	8.15E-07	6.09E+04	5.6	5.0	1.13
40	2.71E-06	2.11E+04	6.6	5.7	1.15
50	6.87E-06	6.89E+03	5.3	4.7	1.13
60	1.47E-05	4.29E+03	7.4	6.3	1.17
80	4.88E-05	1.86E+03	11.5	9.1	1.27
100	1.24E-04	8.51E+02	14.0	10.5	1.33

The strains to failure are small for small stress and larger for medium values of stress. The parameters of Monkman-Grant equation are β=0.849 and C=0.415. This indicates that modelled mechanism is more brittle than in experiment, but the Monkman-Grant constant is comparable with experimental one for stresses in range 30-80 MPa. The influence of failure mechanisms on values of damage tolerance parameters is also visible.

5. CONCLUSIONS

The applied CAFE methodology combines two methods of modelling in different scales. The process of ductile failure is modelled by FE program and brittle failure by CA simulation. The comparison of results with experiment shows that for mixed-mode failure, where both of models interplay, the agreement is satisfactory. For limiting cases, where one of two mechanisms dominates, only some divergence with experiments is observed. It seems that better accordance with brittle failure can be achieved by accurate tuning of CA parameters, whereas model of another mechanism is needed for ductile failure. It seems that it can be achieved by simulation of transgranular voids development.

The CAFE results are in accordance with Kachanov-Hoff theory. An insight into microstructure allowed to obtain finite strains to failure but comparison with experimental values was not possible due to lack of data. Despite of the same structure that was examined the results for all stresses exhibit random character. In the framework of continuum mechanics only agreement of mean experimental data can be achieved. Using Cellular Automata it is possible to examine the microstructure influence on creep failure behaviour what is a subject of further investigations.

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MIKRO- A MAKRO-MODEL ZNISZCZENIA W WARUNKACH PEŁZANIA

Streszczenie

W pracy kontynualne podejście do modelowania przejścia pomiędzy kruchym a ciągliwym zniszczeniem w warunkach pełzania zostało zastąpione poprzez użycie automatu komórkowego. Pozwoliło to na opis tego skomplikowanego zjawiska poprzez nawiązanie do zmian mikrostruktury materiału.

W poprzednich pracach autora technika automatów komórkowych została zastosowana do modelowania struktury materiału i inicjalizacji zniszczenia kruchego. Ta sama metoda została

użyta w obecnej pracy, w której zniszczenie kruche i ciągliwe są równouprawnione. Teoria zniszczenia ciągliwego Hoffa została zaimplementowana przy pomocy pakietu Abaqus i sprzężona z modelem zniszczenia kruchego realizowanym przez automat komórkowy. W ten sposób zaproponowana metoda zawiera się w klasie metod CAFE (Cellular Automata Finite Element). Równoległe uruchomienie obu modeli pozwala na efektywne wyznaczenie punktów przejściowych na wykresie logarytmicznym zależności czasu do zniszczenia od naprężenia. Wyniki są porównane z obserwacjami doświadczalnymi zamieszczonymi w literaturze.

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