GRAIN SIZE DEPENDENCE OF CREEP LIFETIME MODELED BY MEANS OF CELLULAR AUTOMATA

Krzysztof NOWAK*

*Zakład Wytrzymałości Materiałów, Wydział Inżynierii Lądowej,
Politechnika Krakowska, ul. Warszawska 24, 31-155 Kraków

kn@limba.wil.pk.edu.pl

Abstract: Grain size dependence of creep is a complex relation. It can be increasing, decreasing or constant function accordingly to current conditions and material. It is a consequence of complex nature of microscopic mechanisms affecting creep. Some of them are analyzed in current paper by means of multiscale model, using simulation of damage development done by cellular automata technique. It was shown that enlarged sizes of grains, which promote development of intergranular microcracks, are compensated by reduced density of voids forming vacancies. Obtained in simulations grain size dependency follows experimentally observed dependency for small grains in dislocation creep range.

1. INTRODUCTION

1.1. Grain size dependency of creep rate

The phenomenon of creep of polycrystalline materials depends on number of parameters describing their microstructure. One of the most important is grain size. The dependency of steady-state creep rate (or minimum creep rate) on grain size was already largely studied. However, no unambiguous formula for this relation was obtained. It appears that many factors like material structure, temperature, loading level and also environment influence this relation (Boettner and Robertson, 1961).

It is known that for dislocation creep of pure metals rate of secondary creep does not depend on grain size (Dobrzański, 1996), but the majority of alloys exhibits minimum for that relation (Wilshire and Palmer, 2002). If the minimum creep rate is described by equation:

$$\dot{\varepsilon}_{\min} = B\sigma^n \left(\frac{1}{d}\right)^p \exp\left(\frac{-Q_C}{RT}\right), \tag{1}$$

where σ is applied stress, T is temperature, d is grain diameter, Q_c is creep activation energy, B, n, p are material constants, R is gas constant, then the grain size dependency is characterized by parameter p. It is equal to about -2 for large grains, i.e. if the grain is larger then the creep rate is larger, too. The grain boundaries form obstacles for dislocation motion therefore large grains (less borders less obstacles) allow for faster creep rate. For small grains p=1, so the dependency is reverse. The grain boundaries are sources of dislocations and vacancies. If the grains are smaller then there are more borders and more dislocations. The dependency is stronger (p=2) for diffusional creep at small loading level (Wilshire and Palmer, 2002).

The alloys exhibit also the dependency of creep index n (Eq. (1)) on grain size: for larger grains the creep rate dependency upon stress is stronger, and the value of n is larger (Wilshire and Palmer, 2002). Accurate tests showed that similar dependency comes out also for copper. E.g. for dislocation creep at temperature about 0,55 T_m (melting temperature) and for stresses larger than 20 MPa the value of index n is larger for larger grain sizes (see Tab. 1).

Tab. 1. Dependency of creep index n on grain size for copper

grain size [μm]	**temperature** [K]	**creep index** n	**reference**
30	723	4.17	Feltham and Meakin, 1959
40	723	4.48	Wilshire and Battenbough, 2007
100	728	5.24	Evans and Wilshire, 1993
450	723	5.84	Pahutova and others, 1971

These results cannot be used for setting the precise relation, as there are differences among laboratories and test conditions, but the tendency is obvious. Additionally, it can be noticed that the creep rate does not depend on grain size for the stress of about 50 MPa, whereas for smaller stress the smaller grain is the larger creep rate occurs.

1.2. Grain size dependency of time and strain to failure

There is much less experimental data for grain size relation of damage development in creep conditions. But, using the Monkman-Grant relation in form (Evans, 1984):

$$\dot{\varepsilon}_{\min}^{\beta} t_f = C, \tag{2}$$

where t_f is time to failure, β and C are material constants, the time to failure can be approximately evaluated. The relation (2) is very well experimentally confirmed, e.g. for copper in large temperature range (Feltham and Meakin, 1959, Wilshire and Battenbough, 2007). The value of β is changing from 0,8 to 1, and C from 0,003 to 0,6. On this basis it can be assumed that the grain size dependency of time to failure is reverse to the grain size dependency of creep rate.

More experimental data are available for the analysis of the strain to failure value. It is influenced to a greater extent by mechanisms of tertiary creep. According to Fleck and others (1970) a critical crack length (Griffith-Orowan) in comparison to grain size is crucial in determination of strain to failure for large grains. A crack can easily develop along one grain facet, but it is more difficult for this crack to pass from one facet to another. Therefore, if grain size is larger than critical size of crack the failure starts at the beginning of third period of creep and strain to failure is small. The mechanism of voids development is more important in determination of strain to failure for small grains (e.g. lesser than 100 μm in 700 K for copper, Fleck and others, 1970). As the participation of grain boundaries in the whole volume is greater for smaller grains and as grain boundaries are main sources of vacancies the volume fraction of voids is greater for them and thus the strain to failure is smaller.

2. MULTISCALE MODEL OF DAMAGE IN CREEP CONDITIONS

Analysis of grain size dependency of time to failure should include a number of mechanisms occurring in microstructure of material and influencing creep rate and damage development. Taking into account even the most important of these like dislocation climbing, pile-ups, annihilations, grain boundary sliding, nucleation and growth of cavities, crack development leads to very complex model and the analysis of it can be very cumbersome. Every mechanism has its own scale relevant to its subject. The size of single dislocation is about 10^{-10} m, void is about 10^{-6} m, grain - 10^{-4} m, and the size of crack can be comparable to size of construction. The proper analysis of grain size dependency requires multiscale modeling: connection of smaller models appropriate for particular scales (Ostoja-Starzewski, 2007). An example of such procedure is CAFE model of creep damage presented by Chrzanowski and Nowak (2009), Nowak (2011) and used in this analysis. This model consists of deformation model in macroscale, defined by Finite Element (FE) method, and damage model in microscale built using Cellular Automata (CA) technique.

Damage development process is the only one modeled here in microscale. As damage is discontinuous, discrete Cellular Automata are chosen as an appropriate tool for this process (Chrzanowski and Nowak, 2010). They allow for simulation in discrete manner of many processes progressing in material structure.

2.1. Microstructure of material

Microscopic processes are modeled within Representative Volume Element (RVE). It is very difficult to define RVE for damage process. According to Lemaitre and Dufailly (1987) it should be from 50 to 500 μm for metals and it is connected with sizes of defects. On the other side it is connected with material structure (e.g. RVE size is equal to 6-7 grains diameters after Hayhurst, 2005). The model analyzing different grain sizes should keep constant size of RVE with varying number of grains.

The polycrystalline structure of material is built in CA mesh using discrete Voronoi tessellation. First, the n_{seed} number of seed points is randomly distributed over RVE. Every seed point has its own state value allowing for differentiate the grains. Next, the grains growing procedure is applied until whole RVE is covered by cells belonging to particular grains. If the linear size of planar RVE is N_0 then mean grain diameter is:

$$d = N_0 \Big/ \sqrt{n_{seed}} \,. \tag{3}$$

Important state of cell to be distinguished by CA is *damage*. *Damaged cells* can move freely like vacancies or can aggregate into voids. Initial number of *damaged cells* is specified in relation to whole volume by parameter f_{v0}. At the beginning the *damaged cells* are distributed randomly over all RVE.

2.2. Damage model

Two main mechanisms of voids growth are implemented: diffusion of vacancies and deformation of material surrounding voids. Diffusional motion of vacancies is modeled by free moves of *damaged cells*. It is implemented In block neighborhood. All cells are divided into 2x2 blocks and *damaged cells* can change its position inside block randomly. In consecutive CA iteration the position of blocks is shifted so the *damaged cells* can move in any direction. If a *damaged cell* reaches another *damaged cell* especially at grain border they may coalescence into void. The process is controlled by surface energy criterion. The diffusion movement is possible only when it does not contribute to the growth of the value of J, defined as:

$$J = w_{d-m} l_{d-m} + w_{g-g} l_{g-g} \,, \tag{4}$$

where $l_{d\text{-}m}$, $l_{g\text{-}g}$ are lengths of borders between *damaged* and *undamaged* cells, and between two neighboring grains, respectively; $w_{d\text{-}m}$, $w_{g\text{-}g}$ are weight coefficients for these kinds of borders. To promote stability of the method the lengths are calculating in blocks enlarged by one cell in all directions (4x4). The diffusion rate is changed by T_{step} parameter. It is time period (in seconds) equivalent for one diffusion iteration.

The size of RVE is changed according to applied deformation. At beginning of every CA iteration this external deformation is compared with current size of RVE. If deformation exceeds the current size then dimensions of RVE measured in cells are changed accordingly. The deforma-

tion is stretched over cells according to procedure proposed by Matic and Geltmacher (2001) adapted to grain structure (Chrzanowski and Nowak, 2007). The grain boundaries are considered as weaker than grain interior stimulating development of intergranular cracks. Another mechanism connected with deformation is introduced by control of voids volume fraction. Precise density measurements show that it is decreasing with increasing creep strains (Boettner and Robertson, 1961). It is due to development of oids and changes of void volume fraction can be calculated from relative density changes. The strain dependency of void volume fraction (Eq. 5) proposed by Belloni and others (1977) is used in current model to control the number of *damaged cells* during deformation of RVE:

$$\rho = \rho_0\left(1 - H\varepsilon^{\gamma}\right), \tag{5}$$

where ρ, ρ_0 are mass density and initial mass density, ε is strain, H and γ are material parameters. The number of *damaged cells* related to deformation is very important for damage development process. When there are too little *damaged cells* then the effect of inhibited void growth is reached, but when there are lots of *damaged cells* the void growth is enhanced by deformation. In that way it simulates the real material behavior.

The aim of CA model is to determine the value of damage parameter (ω) as homogenized value for RVE. It is calculated as the maximum ratio of linear size of connected path of *damaged cells* to current size of RVE. The RVE is consider as fully damaged when damage parameter is equal to 1 and path of *damaged cells* joins two opposite sides of RVE.

2.3. Deformation model

Macroscopic strains are sum of instantaneous strains and creep strains. Creep strains are obtained numerically by FE method for constitutive equation (Nowak K., 2011):

$$\dot{\varepsilon}_c = B_1\varepsilon_c^{-2}\left(\frac{\sigma\left(1-\omega_0\right)}{1-\omega}\right)^{n_1}, \tag{6}$$

where ε_c is creep strain, σ is stress, B_1, n_1, ω_0 are parameters of deformation model. Damage parameter ω is obtained from CA model running in every Gauss point of FE mesh. Strains calculated according to Eq. (6) are used to determine current size of RVE in CA model. Parameters B_1, n_1 are fitted to primary period of creep curve, where damage can be neglected for real material. Parameter ω_0 in Eq. (6) compensates non-zero initial value of damage for CA model. It was necessary because non-zero initial value of f_{v0} parameter and large instantaneous (plastic) strain produce significant value of damage parameter already in early stages of simulation. The final failure is assumed when damage parameter reaches 1 in any Gauss point.

3. RESULTS

Analysis of grain size dependency has been performed using model described above. The model parameters have been suited to the results of creep experiment for copper in 823 K for grain size of 30 μm (Feltham and Meakin, 1959). The deformation model parameters were as follows: B_1=7.57E-24 (MPa)^{n_1}s^{-1}, n_1=9.76, ω_0=0.15. They were calculated from values of β parameter of primary strain equation reported by Feltham and Meakin (1959):

$$\varepsilon_c = \beta t^{1/3}, \tag{7}$$

where t is time.

The model uses structure described by N_0=641, n_{seed}=10. According to Eq. (3) it gives mean grain diameter d=202.7 cells. By comparison to experimental grain size (30 μm) the size of single cell can be estimated as 0.15 μm and RVE size as nearly 100 μm. The size of single cell can be regarded as size of smallest recognized void. The model of intergranular failure is implemented and voids can develop only along grain boundaries: $w_{d\text{-}m}$=0, $w_{g\text{-}g}$=1. Parameters of Eq. (5) were set to H=1.17 and γ=2.3. They were obtained by regression analysis of data for copper in temperatures 673 K - 823 K and stress range 21 MPa - 34 MPa (Boettner and Robertson, 1961). Remaining parameters of damage model were suited to secondary creep data: f_{v0}=0.006, T_{step}=0.25 s (see Fig. 1). The agreement of times to failure and strains to failure with experimental data was obtained.

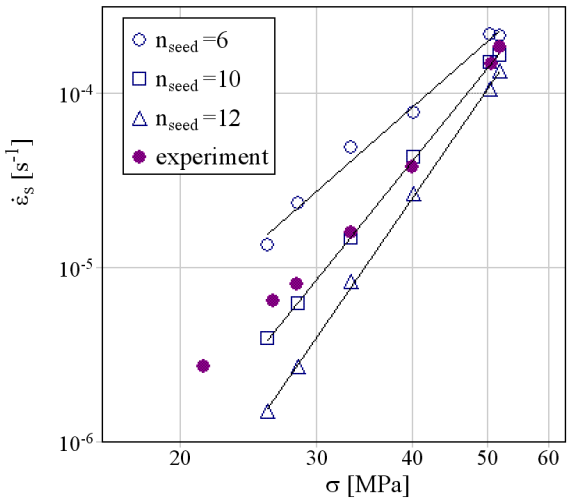

Fig. 1. Dependency of stationary creep rate on parameter n_{seed} – simulation results in comparison with experimental results (Cu at 823 K 30 μm mean grain size, Feltham and Meakin, 1959)

Next, the influence of parameter n_{seed} was examined. The simulations were performed for n_{seed}=6, 10 and 12, keeping other parameters constant (see Fig. 1). It corresponds to grain sizes: 39, 30, 27 μm. The creep rates are decreasing for decreasing grain sizes and the creep indexes n (Eq. 1) calculated as tangent of regression line at Fig. 1 are increasing (3.89, 5.49, 6.45, accordingly).

Results for time to failure are compatible with experimental relation (2). Times to failure are larger for smaller grains and the difference is greater for smaller stresses. This behavior is typical for large grain sizes as damage is growing faster for larger grains. The diffusion mechanism

of void growth is prevailing for small stresses and number of *damaged cells* in relation to lengths of all borders in RVE becomes deciding parameters in damage development simulation.

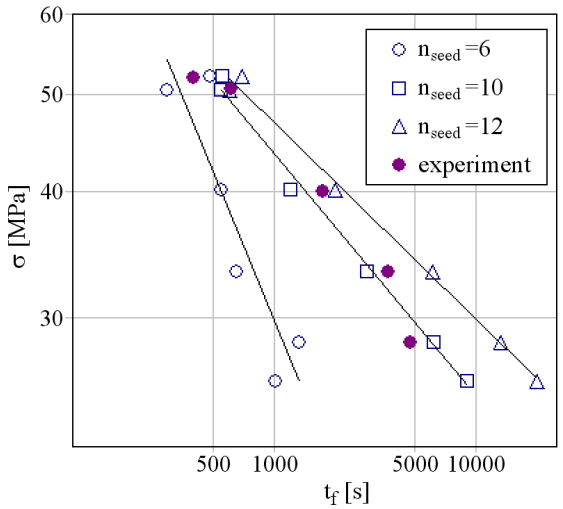

Fig. 2. Dependency of time to failure on parameter n_{seed} – simulation results in comparison with experimental results (Cu at 823 K 30 μm mean grain size, Feltham and Meakin, 1959)

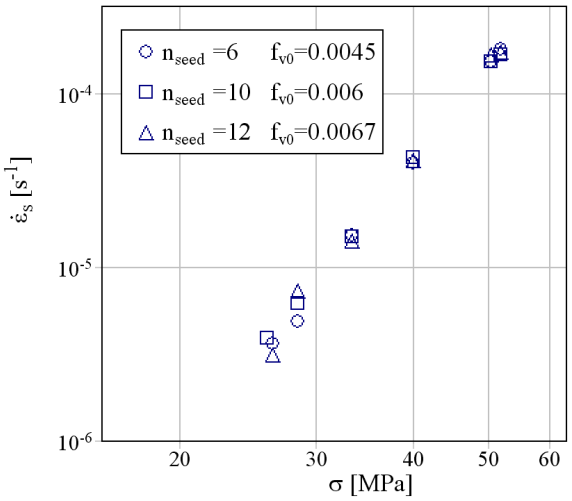

Fig. 3. Dependency of stationary creep rate on parameters n_{seed} and f_{v0} – simulation results

In real materials number of vacancies is connected with surfaces of grain boundaries as grain boundaries are ideal sources of vacancies (Evans, 1984). Therefore, smaller grains have increased number of vacancies. To reflect this effect the initial density of *damaged cells* f_{v0} has to be corrected. For 3D model of constant RVE size, number of grains is changing like $\sim d^{-3}$, surface of single grain boundaries is like $\sim d^{2}$, so surface of all grains in RVE is $\sim d^{-1}$. Similarly for 2D model: number of grains is changing like $\sim d^{-2}$, length of single grain boundaries is like $\sim d$, so length of all grains borders in RVE is $\sim d^{-1}$. In all cases, to keep the value of f_{v0} proportional to the length (or surface) of grain boundaries it should be $\sim d^{-1}$. The value of parameter H (Eq. 5) is changed in the same proportion, too.

Results of simulations with corrected values of f_{v0} are presented on Figs 3 and 4. Obtained creep rates coincide very well, showing that there is no dependency of creep rate on grain size. The larger value of f_{v0} fully compensates the smaller size of grains. This is consistent with general relation for metals in dislocation creep range. The results for time to failure exhibit more scatter, but there is also no apparent dependency on grain size. The results of simulation comply with the Monkman-Grant rule (2).

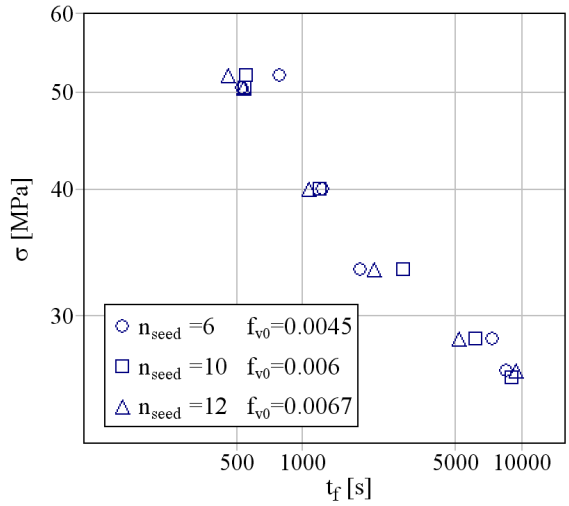

Fig. 4. Dependency of time to failure on parameters n_{seed} and f_{v0} – simulation results

4. CONCLUSIONS

The simulations of damage development in creep conditions by means of Cellular Automata show that the simple enlargement of grains is not sufficient to explain observed experimentally dependency on grain size. Besides grain size also initial density of *damaged cells* is important to properly simulate this dependency. But comparison with the experiments for copper (see Tab. 1) shows that not all mechanisms connected with grain size are taken into account and thus further investigation has to be performed.

REFERENCES

1. **Abedrabbo N., Pourboghrat F., Carsley J.** (2006), Forming of AA5182-O and AA5754-O at elevated temperatures using coupled thermo-mechanical finite element models, *International Journal of Plasticity*, 23, 841–875.
2. **Bolkowski S., Stabrowski M., Skoczylas J., Sroka J., Sikora J., Wincenciak S.** (1993), *Komputerowe metody analizy pola elektromagnetycznego*, WNT, Warszawa.
3. **Goshima T., Hanson M.T., Keer L.M.** (1990), Three-dimensional analysis of thermal effects on surface crack propagation in rolling contact, *Journal of Thermal Stresses*, Vol. 13, 237-261.
4. **Grześ P.** (2009), Finite element analysis of disc temperature during braking process, *Acta Mechanica et Automatica*, Vol. 3, No. 4, 36-42.

5. **Kaczorek T.** (2002), *Positive 1D and 2D Systems*, Springer Verlag, London.
6. **Malinin N. N, Rżysko J.** (1981), *Mechanika materiałów*, PWN, Warszawa.
7. **Belloni G., Bernasconi G., Piatti G.** (1977), Creep damage and rupture in AISI 310 austenitic steel, *Meccanica*, Vol. 12, 84-96.
8. **Boettner R.C., Robertson W.D.** (1961), A Study of the Growth of Voids in Copper During the Creep Process by Measurement of the Accompanying Change in Density, *Trans. Metall. Soc. AIME*, Vol. 221, 613-622.
9. **Chrzanowski M., Nowak K.** (2007), Cellular Automata in Damage Mechanics: Brittle Creep Rupture Case, *Arch. Mech.*, Vol. 59, 329-339.
10. **Chrzanowski M., Nowak K. (**2009), On Multiscale Modelling of Creep Damage by Means of Cellular Automata, *Journal of Multiscale Modelling*, Vol. 1, 389-402.
11. **Chrzanowski M., Nowak K. (**2010), Opis zniszczenia mieszanego w warunkach pełzania przy pomocy automatów komórkowych, *Acta Mechanica et Automatica*, Vol. 4, 29-36.
12. **Dobrzański L.A. (**1996), *Metaloznawstwo z podstawami nauki o materiałach*, Wydawnictwa Naukowo-Techniczne, Warszawa.
13. **Evans H.E. (**1984), *Mechanisms of Creep Fracture*, Elsevier Applied Science Publishers, London, New York.
14. **Evans R.W., Wilshire B. (**1993), *Introduction to Creep*, The Institute of Materials, London.
15. **Feltham P., Meakin J.D. (**1959), Creep in Face-Centred Cubic Metals with Special Reference to Copper, *Acta Metall*., Vol. 7, 614-627.
16. **Fleck R.G., Cocks A.C.F., Taplin D.M.R. (**1970), The Influence of Polycrystal Grain Size upon the Creep Ductility of Copper, *Metall. Mater. Trans.*, Vol. 1B, 3415-3420.
17. **Hayhurst D.R.** (2005), CDM mechanisms-based modelling of tertiary creep: ability to predict the life of engineering components, *Arch. Mech.*, Vol. 57, 2-3.
18. **Johnson W. R., Barrett C.R., Nix W.D. (**1972), The effect of environment and grain size on the creep behavior of a Ni-6 pct W solid solution, *Metall. Mater. Trans.*, Vol. 3B, 695-698.
19. **Lemaitre J., Dufailly J.** (1987), Damage measurements, *Eng. Fract. Mech.*, Vol. 28, 643-661.
20. **Matic P., Geltmacher A.B.** (2001), A cellular automaton-based technique for modeling mesoscale damage evolution, *Comp. Mat. Sci.*, Vol. 20, 120-141.
21. **Nowak K. (**2011), Uncertainty of lifetime for CAFE creep damage model, *Computer Methods in Materials Science*, Vol. 11, 315-323.
22. **Ostoja-Starzewski M. (**2007), *Microstructural Randomness and Scaling in Mechanics of Materials*, Chapman and Hall/CRC.
23. **Pahutova M., Cadek J., Rys P. (**1971), High temperature creep in copper, *Phil. Mag.*, Vol. 22, 509-517.
24. **Wilshire B., Battenbough A.J. (**2007), Creep and creep fracture of polycrystalline copper, *Mater. Sci. Eng.*, Vol. 443A, 156-166.
25. **Wilshire B., Palmer C.J. (**2002), Grain size effects during creep of copper, *Scripta Mater.*, Vol. 46, 483-488.