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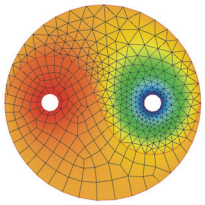

# MODELLING OF BRITTLE DAMAGE NUCLEATION BY MEANS OF CA

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**Abstract**

The description of damage nucleation in metals subjected to creep conditions, on the level of material structure, is proposed. In classical approach of mechanics it is achieved by introducing scalar (or tensorial) parameter called damage variable and postulating the phenomenological equation of its evolution. Such an approach has been successfully used in analysis of structures under different loading circumstances, giving rise to the formation of special branch of mechanics called "Continuum Damage Mechanics" (CDM). In spite of achieving numerous solutions to important technical problems, like estimation of the time to the appearance of first macroscopic defect, and further development of cracking process, this approach reflects neither physical process that is underlying macroscopically observed phenomena, nor material structure. In the present paper a multiscale approach is proposed by combining numerical solution on macroscopic level with microscopic behaviour of a particular material structure using Cellular Automata. The solutions of analyzed problems are compared with those obtained by means of CDM.

**Key words**: cellular automata, brittle creep fracture, damage mechanics

## 1. FRACTURE IN CREEP CONDITIONS

### 1.1. Macroscopic observations level

The process of material deformation in creep conditions is well recognised on macroscopic level of observation. The phenomenological laws bonding stresses and strains (or their time derivatives) are formulated in frame of continuum mechanics and can be written in form of equations:

$$F(\varepsilon_{ij}, \sigma_{ij}, t) = 0, \tag{1}$$

where $\varepsilon_{ij}$ is strain, $\sigma_{ij}$ – stress tensor, t - time. These equations do not constitute time limit for the creep process. On the other hand the deformation process is associated with progressive deterioration of material structure. In continuum mechanics new state variable responsible for damage phenomenon (microdefects of material structure) is introduced. It is achieved through homogenisation of microdefects over Representative Volume Element (RVE).

Damage variable, in general of tensorial character, has to be governed by an evolution law. Such a law was proposed by L. M. Kachanov (1958) using scalar measure of damage variable $0 \leq \omega \leq 1$. It gave rise to a new branch of mechanics– Continuum Damage Mechanics (CDM) (Janson & Hult, 1977). It has been proved that CDM is able to successfully describe both the process of deformation and deterioration, cf. monographs by Lemaitre (1992), Krajcinovic (1996), Skrzypek & Ganczarski (1999). A number of the solutions to practical problems were also achieved.

As a reference solution to the proposed method we use the following set of evolution laws for deformations and deteriorations (after Bodnar & Chrzanowski, 2002):

$$\varepsilon_{ij} = \varepsilon^{e}_{ij} + \varepsilon^{c}_{ij}, \tag{2}$$

$$\varepsilon^{e}_{ij} = D^{-1}_{ijkl}\,\sigma_{kl}, \tag{3}$$



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$$\frac{\partial \varepsilon_{ij}^{c}}{\partial t} = \gamma \left( \frac{\sigma_{eff}}{1-\omega} \right)^{n} \frac{\partial \sigma_{eff}}{\partial \sigma_{ij}}, \qquad (4)$$

$$\frac{\partial \omega}{\partial t} = A \left[ \alpha \frac{\sigma_{max}}{1-\omega} + (1-\alpha) \frac{\sigma_{eff}}{1-\omega} \right]^{m}, \qquad (5)$$

where: $\varepsilon_{ij}$, $\varepsilon_{ij}^{e}$, $\varepsilon_{ij}^{c}$ - total, elastic and creep strain tensors, respectively, $\sigma_{ij}$ - stress tensor, $D_{ijkl}$ - elastic constants matrix, $\gamma$, n, A, m, $\alpha$ - steady-state creep and damage material constants, $\sigma_{max}$, $\sigma_{eff}$ - main positive principal stress and Huber-Mises effective stress, respectively, $\omega$ - scalar damage parameter ($0 \leq \omega \leq 1$), t - time.

### 1.2. Microscopic observations level

For metals the development of structure deterioration is a subject of numerous investigations. Different mechanisms of this process are conventionally summarised on so called damage maps (figure 1).

In this paper we consider intergranular creep fracture which has two forms: voids and triple point cracks at grain boundaries. This process occurs at high temperatures and low stresses: the temperature is about 60% of melting point and the stress is below 10% of yields strength. The time to failure is rather very long (years) and strains at failure relatively small of order of several percents. As this type of failure occurs at grain boundaries (figure 2) it is necessary to model material structure to capture the most characteristic feature of this process.

## 2. APPLICATION OF CELLULAR AUTOMATA

Both grain boundaries and voids or cracks are discontinuous and to model their influence on microscopic mechanisms the tool which supports discontinuous calculations is needed. There are many applications of CA in modelling of metallurgy processes like recrystallisation, solidification or metal formation (Gawąd et al., 2005). Some applications also deal with the problem of material damage. The mass conservation law to model damage growth was used by Matic & Geltmacher (2001). Combination of Finite Element Method and CA was recently introduced (cf. e.g. Shterenlikht & Howard, 2004) to facilitate multiscale modelling. The present paper falls into the frame of this approach.

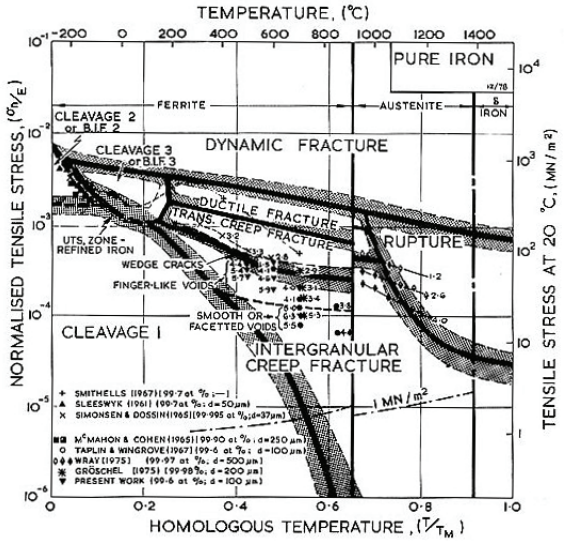


***Fig. 1.*** *Fracture mechanism map for pure iron (NIST, 2001).*

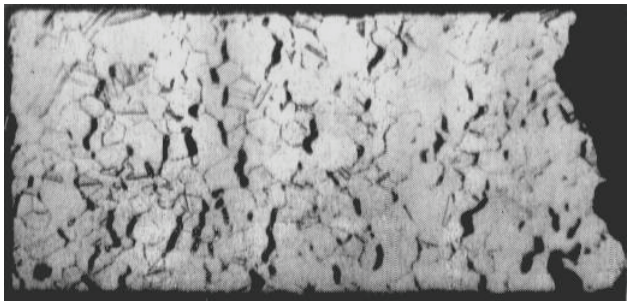

***Fig. 2.*** *Commercial brass: 6% creep in °400C (Hans, 1961).*

### 2.1. Definitions

To define the cellular automaton one has to state (Kułakowski, 2000):

- a network of cells in D-dimension space;
- a set of possible states of a cell;
- rules governing the state of a cell in time *t+1* depend on the state of the cell and its neighbourhood in time *t*.

For the purpose of this work, the cellular automaton was developed, but slightly different from the classical definition above, as the rule governing the state depends also upon some global variables.

It uses the 2D network of cells, theoretically stretching to infinity, but for practical needs (memory consumption) limited to a finite number. The set of possible states is: $\{-1,0,1,...,N_{grains}\}$. Number -1 denotes the cell outside of modelled RVE; 0 – the **empty cell** inside modelled RVE; $1,...,N_{grains}$ are the numbers of grains to which the cell belongs to, a cell with such a state is called a **mass cell**. The model of RVE has some initial size in cells - $N_{init}$, and is assumed to be a square. The size of RVE is always an odd number. The numbering of cells is as follows: the central cell has indices (0,0) and the network



extends in four directions, so the indices of corners of RVE are (-n, n), (n, n), (-n,-n), (-n, n), where n= ($N_{init}$-1)/2. Such a numeration allows to change the total number of cells easily and assures clear deformation procedure, as deformation is always symmetrical.

The automaton uses several rules depending on the stage of automaton and process parameters. The used rules are probabilistic ones, and as it was stated earlier, the new state of cell depends on the cell state itself, its neighbours, and some global parameters. All rules use Moore neighbourhood.

As the modelled process is complex, the rules are divided into two procedures:
- material structure formation,
- damage growth.

### 2.2. Modelling of structure

The most popular procedure for modelling granular structure in continuous space is the Voronoi tessellation. The definition of it can be as follows:

$$x \in X \Leftrightarrow d(x, seed(X)) < d(x, seed(Y)), \quad (6)$$

where: x – any point, X –grain, Y - any other grain, seed() – is function returning the seed point of grain, d – distance measure. The tessellation proposed here (after Adamatzky, 1996) uses the definition based on discrete measure of distance in terms of Moore neighbourhood:

$$d(x, y)=\min(|x_1-y_1|,|x_2-y_2|), \quad (7)$$

where x, y are discrete points (or cells) with coordinates $(x_1,x_2)$, $(y_1,y_2)$.

The first stage of process - grains initiation comprises selection of seeds points for grains. For this purpose the homogenous Poisson point process is used with chosen seed point number $n_{seeds}$. Only the initial volume of RVE is seeded with these points. The grain number is chosen randomly for every seed point. It can happen that two seed points have the same grain number and grains raised from such points merge into one grain if they are close enough. The average initial size (in cells) of grains is

$$d_{grain}=N_{init} / n_{seeds}^{½} \quad (8)$$

The second stage of structure modelling is a procedure for grains formation. It is governed by a simple rule defining the function of the cell state:

$$F(x,t+1)=\left\{\begin{array}{c} F(x,t) \\ \text{mean}(F(y,t): y \in \text{Neighourhood}(x) \text{ and } F(y,t)\neq 0) \end{array} \text{ if } \begin{array}{c} F(x,t)\neq 0 \\ F(x,t)=0 \end{array}\right\} \quad (9)$$

where mean is function returning mean value rounded to the closest integer. The rule is executed until all volume of RVE is filled with mass cells.

Thanks to this rule the shape of grains can be both: convex or concave, in contradiction to classical Voronoi tessellation. The second property is that some grains do not have their seed points, they are formed along boundaries of other grains in long, narrow shapes. The typical tessellation is shown in figure 3.

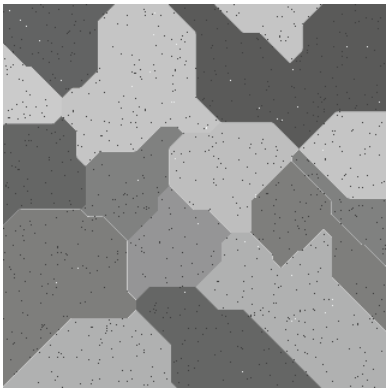

***Fig. 3.*** *Typical initial structure for $n_{seeds}$=20 with damage density $g_{dam0}$=0.01.*

The grain number is introduced only to distinguish different grains, there is no connection between this number and any other grain properties such as orientation. These properties of grains are not taken into account in the present analysis, as only intergranular failure is considered.

Modelling of structure includes also the procedure of initial damage distribution. It is assumed that it is a homogenous Poisson point process with density $g_{dam0}$. The initial damage is necessary for the damage development procedure to run (see next section).

All above procedures are needed only to construct the initial material structure. So for all these procedures $t<t_0$. The loading starts at $t_0$ and the next section describes time dependent procedures under external load.

### 2.3. Modelling of damage growth

The main rule governing cellular automaton behaviour in this stage is the mass conservation law. It is the global law that controls the number of all mass cells in automaton:



$$M(t)=count(x: F(x, t)>0)=const(t)=M(t_0)=M_0, \quad (10)$$

count() is function counting the number of the set elements.

The consequence of this law is the total number of empty cells. If V(t) is the volume of RVE in number of cells in time step t and E(t) is the number of empty cells then obviously:

$$M(t)+E(t)=V(t) \quad (11)$$

and

$$E(t)=V(t)-M_0=V(t_0)+\Delta V(t)-M_0=E(t_0)+\Delta V(t)= V(t_0)\cdot g_{dam0}+ \Delta V(t) \quad (12)$$

and finally

$$\Delta E(t) = \Delta V(t). \quad (13)$$

is projected over CA network. For every cell temporary fractional mass is counted separately for each grain – m(x, t, g), where x is cell, t – time increment, g – grain number. For any x:

$$0 \le \sum_{g=1}^{N_{grains}} m(x,t,g) \le 1 \quad (15)$$

Based on its value the new state of CA cell is calculated following the rule:

$$F(x,t) = \begin{Bmatrix} g_{max}(x,t) & \text{if } m(x,t,g_{max}) > m_{threshold} \\ 0 & \text{elsewhere} \end{Bmatrix}, \quad (16)$$

where $g_{max}(x, t)$ is the number of the grain with maximum value of m(x, t, g).

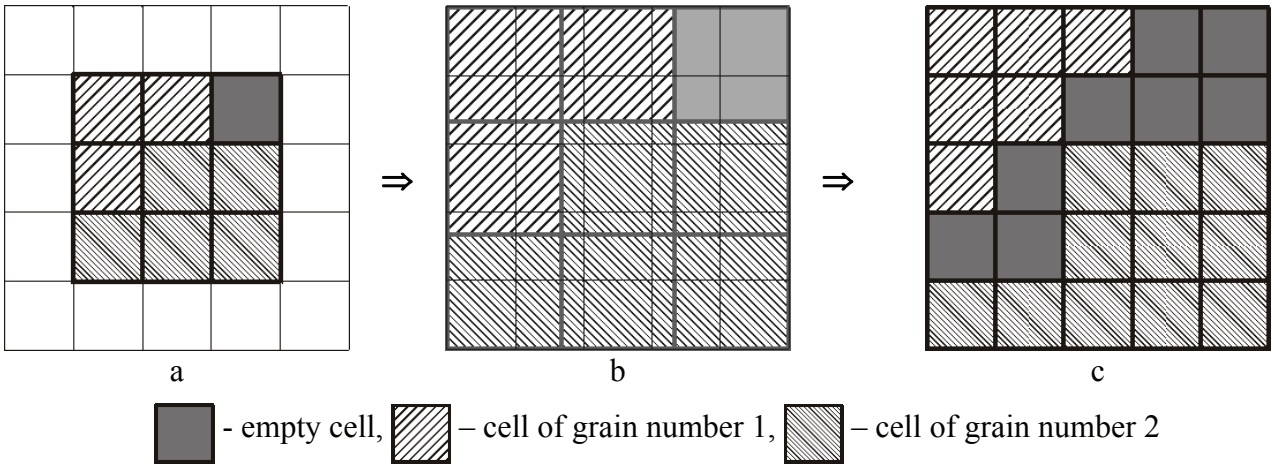


***Fig. 4.*** *Deformation step for 3x3 RVE with two grains.*

The consequence of mass conservation rule is: if volume of RVE is constant then the number of empty cells is constant, too.

The process of damage growth induced by prescribed deformation consists of two steps in each time increment. The first step is deformation or creep step, the second step is damage evolution step. As the total number of empty cells in every time is known, the parameter β is introduced to distinguish number of cells emptied in the first and second steps. Let $E_1(t)$ denote number of empty cells after the first step in time increment t, then the number of empty cells to be created in the second step is:

$$E_2(t)=E(t)-E_1(t), \text{ hence } \beta=E_1(t) / E(t). \quad (14)$$

Deformation step starts with extending or compressing the RVE over one cell in some directions. The changes are assumed to be symmetrical, so if the left side is extending, the right one is extending, too, and so on. After deformation the mass of deformed cells

The threshold value $m_{threshold}$ is calculated in each time increment, based on mass conservation law and parameter β. The values of $m(x, t, g_{max})$ for all mesh cells are ordered from 0 to 1, and then $E_1(t)= \beta\cdot E(t)$ cells are counted, and $m_{threshold}$ is a value of fractional mass of $E_1(t)$ cell.

To illustrate the procedure let us consider the simplified example (figure 4).

RVE is assumed to be in $t_0$ 3x3 cells. Cell (1,1) is empty, cells (-1,1),(0,1),(-1,0) belong to grain number 1, the remaining cells belong to grain number 2. The RVE is extended by 1 cell in all directions, over 5x5 mesh (figure 4b). The fractional mass is calculated for all cells in time $t=t_0+1$. Results for cells on boundaries are summarized in table 1, the remaining cells have fractional mass for $g_{max}$ equal to 1:

In example $M_0=8$, so E(t)=25-8=17. If we suppose that β= 0.5 then $E_1(t)=int(0.5\cdot 17)=8$. From table 1 we obtain that $m_{threshold}=7/9$. Final result of deformation procedure is in figure 4c.



***Table 1.*** *Calculation of threshold value. Cells are ordered according to increasing value of $m(x,t,g_{max})$.*

| order no | x | m(x,t,1) | m(x,t,2) | $g_{max}(x,t)$ | F(x,t) |
|---|---|---|---|---|---|
| 1 | (2,2) | 0 | 0 | - | 0 |
| 2 | (1,2) | 1/3 | 0 | 1 | 0 |
| 2 | (2,1) | 0 | 1/3 | 2 | 0 |
| 2 | (1,1) | 2/9 | 1/3 | 2 | 0 |
| 5 | (0,1) | 2/3 | 1/3 | 1 | 0 |
| 5 | (-1,0) | 2/3 | 1/3 | 1 | 0 |
| 5 | (-2,-1) | 1/3 | 2/3 | 2 | 0 |
| 8 | (-1,-1) | 2/9 | 7/9 | 2 | 0 |
| 9 | (-1,1) | 8/9 | 1/9 | 1 | 1 |

In the above example the prescribed strain is 67%. In real brittle creep process the strains at failure are of the order of several percent, so much bigger mesh is needed.

If the large network is deformed, some mesh correlation effect is observed. The state of side and central cells changes very little, and the cells in half distance from the centre to the side change a lot. To avoid it some random values in deforming the mesh are introduced. If $k_i$ is deformation factor in i direction, then $k_i=N_i(t+1)/N_i(t)$, where $N_i(t)$ is the size of RVE in i direction. The coordinates of deformed mesh in temporary state are

$$x_i^*(t+1)=x_i(t)\cdot k_i+r, \qquad (17)$$

r is random number with uniform distribution from -0.5 to 0.5.

The same decorrelation mechanism is used in so-called diffusion step, when creep process is controlled by diffusion process depending on time and temperature growth. To account for this effect the physical time of the process is discretised upon the basis of $T_{diff}$ parameter. The smaller the temperature the higher the value of $T_{diff}$ parameter, and consequently more time steps are allowed for development of diffusion. The diffusion step is performed in the same way as deformation step but without the external deformation ($k_i=1$). The coordinates of temporary cells for this process are:

$$x_i^*(t+1)=x_i(t)+r. \qquad (18)$$

The second step in each time increment is damage evolution step. To obtain the number of empty cells according to mass conservation a probabilistic rule is used. First a mean probability $p_0$ is calculated. As mass $M_1(t)$ after deformation step is greater than initial mass $M_0$ (which has to be constant in all time increments) then the probability that mass cell becomes an empty cell in the second step is:

$$p_0=\frac{E_2(t)}{V(t)-E_1(t)}=\frac{M_1(t)-M_0}{M_1(t)}, \qquad (19)$$

$M_1(t)$ is the number of mass cells after the first step. Then some weights are used to model the influence of neighbouring cells. If z denotes the type of neighbourhood then the probability of mass cell with neighbourhood z to become an empty cell is:

$$p_z=p_0\cdot W_z. \qquad (20)$$

The weights $W_z$ depend on the type of neighbourhood.

At the end of each time increment the evaluation of damage variable is performed. To calculate the damage value the maximum size of areas of the connected empty cells is searched. This maximum size is calculated separately in both directions and then divided by the actual size of RVE in that direction. The largest of such calculated values is used as scalar damage variable. When this variable reaches 1 the size of connected empty cells is equal to the size of RVE. In this situation i.e. when the empty cells form a path spanning opposite sides of RVE, the element is considered to be destroyed, and becomes a nucleus of macroscopic crack.

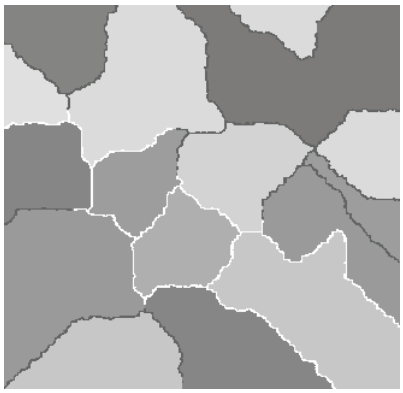

***Fig. 5.*** *Path of empty cells spanning sides of RVE (in white). Remaining empty cells are black.*

## 3. MULTISCALE MODELLING

### 3.1. CAFE methodology

To bridge the microstructural changes with macroscopic behaviour of a structure, the CAFE methodology is used. First finite element calculations for modelled structure are performed using equations (2)-(4), then deformation in Gaussian points are dealt with CA as prescribed deformation for RVE in this point. The procedure for damage growth starts if deformation is greater than 2 cells of RVE (value $2/N_{init}$ is deformation resolution of automaton) or when time reaches the value for diffusion step – $T_{diff}$. After CA calculations the damage variable is re-



turned to finite element code and used in equation (4) in the next time increment.

### 3.2. Example of biaxial tension of creeping plate

As an example the behaviour of creeping plate under biaxial tension is modelled. For analysis the finite element program ABAQUS is used. The constitutive equations and cellular automata are implemented in user subroutine UMAT. The results obtained from CA are compared with CDM solution for Ti-6Al-2Cr-2M alloy at temperature 675 K. The materials constants are $E=0.102\cdot10^6$ MPa, $\nu=0.33$, $n=6.8$, $\gamma=1.38\cdot10^{-24}$ $(MPa)^{-n}h^{-1}$, $m=5.79$, $A=1.08\cdot10^{-20}$ $(MPa)^{-m}h^{-1}$ (Walczak & Sieniawski, 1983).

In CA calculation the following parameters are used: $N_{init}=321$, $n_{seeds}=20$, $N_{grains}=10$, $T_{diff}=1e6$, $\beta=0.85$, $g_{dam0}=0{,}01$. The results are shown in table 2, where time to first macroscopic defect for CDM FE and CA solutions are compared.

***Table 2.*** *Time to first macroscopic defect for biaxial tension.*

| $p_1$ [MPa] | $p_2$ [MPa] | t* [h] CDM FE | | | t* [h] CAFE |
|---|---|---|---|---|---|
| | | α=0 | α=0.5 | α=1 | |
| 100 | 0 | 8,47E+07 | 5,69E+07 | 3,98E+07 | 1,61E+08 |
| 100 | 10 | 1,54E+08 | 7,58E+07 | 4,22E+07 | 2,94E+08 |
| 100 | 20 | 3,00E+08 | 1,03E+08 | 4,54E+07 | 6,09E+08 |
| 200 | 0 | 1,53E+06 | 1,03E+06 | 7,18E+05 | 2,22E+06 |

## 4. CONCLUSIONS

It was demonstrated that the procedure used in the paper enabled description of multiscale modelling of brittle failure of polycrystalline materials in creep conditions. The coupling of FEM and CA resulted in realistic description of complex process of material deterioration, which takes place along grain boundaries.

Further development of the model should cover influence of grains orientation and their properties, which is of importance in the case of transgranular failure. This should also shorten the time to failure, which in the present analysis is one order higher than that of classical CDM solution.

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### MODELOWANIE NUKLEACJI USZKODZEŃ KRUCHYCH PRZY POMOCY AUTOMATÓW KOMÓRKOWYCH


Streszczenie

Zaproponowano opis nukleacji uszkodzeń dla metali pracujących w warunkach pełzania na poziomie mikrostruktury. Opisując to zjawisko w klasycznym podejściu do mechaniki wprowadza się skalarny (lub tensorowy) parametr nazywany uszkodzeniem i postuluje fenomenologiczne prawo jego rozwoju. Takie podejście jest z powodzeniem używane w analizie konstrukcji w różnych warunkach obciążenia tworząc specjalną gałąź mechaniki zwaną kontynualną mechaniką uszkodzeń. Pomimo rozwiązania szeregu ważnych technicznych problemów, takich jak oszacowanie czasu do pojawienia się pierwszego makroskopowego uszkodzenia a także dalszego rozwoju procesu pękania, podejście to nie odzwierciedla ani procesu fizycznego leżącego u podstaw makroskopowo obserwowanych zjawisk, ani struktury materiału. W niniejszej pracy proponuje się podejście wieloskalowe poprzez połączenie rozwiązania numerycznego na poziomie makroskopowym z opisem zachowania się struktury materiału na poziomie mikro przy pomocy automatów komórkowych. Otrzymane rozwiązania porównane są z rozwiązaniami otrzymanymi przy pomocy kontynualnej mechaniki uszkodzeń.



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