Micro scale modeling of grain boundary damage under creep conditions

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Introduction. Constitutive modeling of high-temperature creep of modern materials under complex loading requires understanding of micromechanical processes, taking place on the level of grains. To achieve this, creep damage simulation on microlevel is performed. Following processes are investigated: power law creep within the grain, grain boundary sliding and grain boundary cavitation.
In automotive industry electronic devices with the dimensions of several millimeters are often used in last decades. Such devices placed near the engine undergo high-temperature deformations. Due to their size, creep processes have to be simulated, taking into account material heterogeneity.

Problem Definition

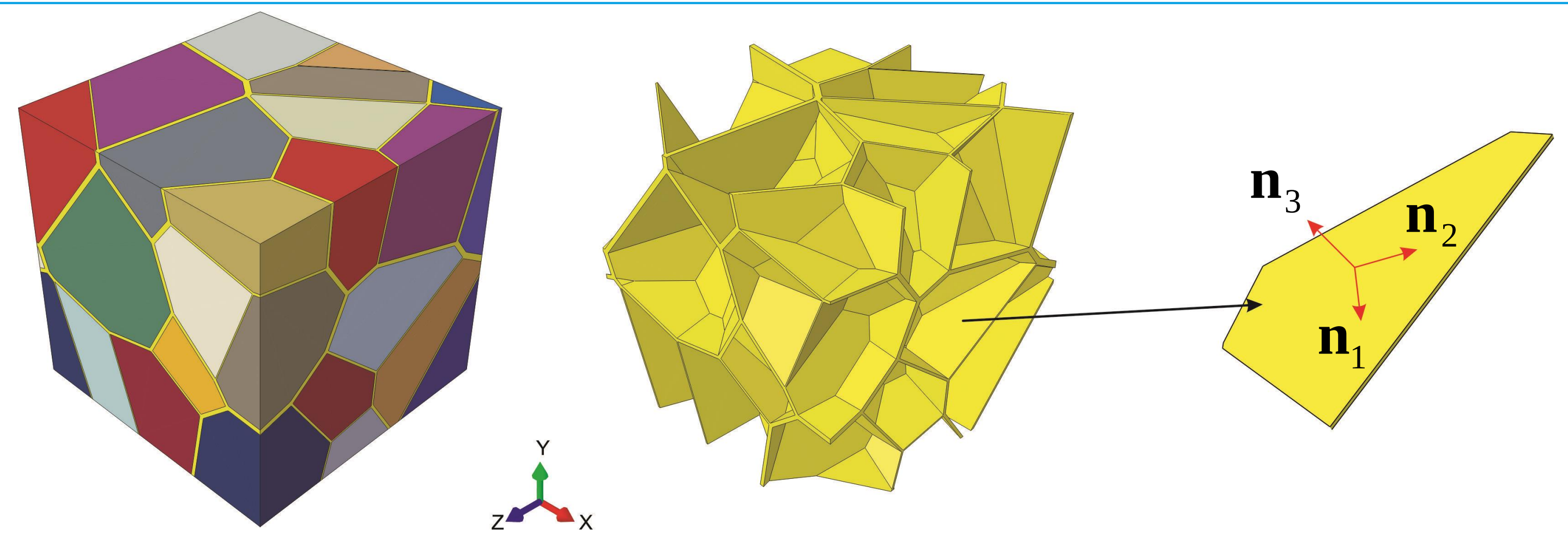
Creep damage analysis of the polycrystalline material on the micro scale in order to investigate influence of elastic and creep deformation of anisotropic grains, grain boundary sliding and grain boundary cavitation on the macroscopic responce.

Cooperation

- Polycrystalline geometry:
Oleksandr Prygorniev and Srihari Dodla;
- Crystal plasticity:
Shyamal Roy, Esmaeil Tohidlou, Dr.-Ing. Rainer Glüge.
- Micrographs of the fractured specimens are performed with with Jun.-Prof. Dr.-Ing. Manja Krüger assistance;

- Uniaxial tensile creep tests under polycrystalline copper at 550 ˚C are performed at the Mechanical Engineering department of University of Milan (Italy) under the supervision of Prof. Elisabetta Gariboldi.

Analytical Description



Geometrical representation of a polycrystal. Unit cell with the grain boundary region, possessing a local material orientation.

- Elastic material behavior of grain interior is assumed to possess cubic symmetry. Whereas grain boundary regions are assigned to orthotropic symmetry. The reasons for this is the necessity to distinguish between the shear and normal deformations in order to reproduce the grain boundary sliding. Dependence of the stress tensor on the elastic strain tensor components for both materials is described by the following orthotropic law:

$$\begin{aligned}\sigma \quad &= \alpha_1^2(\varepsilon_{11}+\varepsilon_{22}+\varepsilon_{33})(\mathbf{n}_1\otimes\mathbf{n}_1+\mathbf{n}_2\otimes\mathbf{n}_2+\mathbf{n}_3\otimes\mathbf{n}_3)\\ &+[\beta_1(\varepsilon_{11}-\varepsilon_{22})+\beta_2(\varepsilon_{11}-\varepsilon_{33})]\mathbf{n}_1\otimes\mathbf{n}_1+[\beta_1(\varepsilon_{22}-\varepsilon_{11})+\beta_3(\varepsilon_{22}-\varepsilon_{33})]\mathbf{n}_2\otimes\mathbf{n}_2\\ &+[\beta_2(\varepsilon_{33}-\varepsilon_{11})+\beta_3(\varepsilon_{33}-\varepsilon_{22})]\mathbf{n}_3\otimes\mathbf{n}_3+2\beta_{12}\varepsilon_{12}(\mathbf{n}_1\otimes\mathbf{n}_2+\mathbf{n}_2\otimes\mathbf{n}_1)\\ &+2\beta_{13}\varepsilon_{13}(\mathbf{n}_1\otimes\mathbf{n}_3+\mathbf{n}_3\otimes\mathbf{n}_1)+2\beta_{23}\varepsilon_{23}(\mathbf{n}_2\otimes\mathbf{n}_3+\mathbf{n}_3\otimes\mathbf{n}_2).\end{aligned}$$

- The material parameter set allows a transition to cubic symmetry case. Parameters are determined from elastic tests of single crystal copper [2] and physical considerations.
- Power law creep is assumed for grain interior material. For case of orthotropy it has the form:

$$\begin{aligned}\dot{\varepsilon}^{\mathrm{c}} \quad &= \frac{a\sigma_{eq}^{n-1}}{2}\Big[\Big(\mathbf{n}_1\otimes\mathbf{n}_1-\frac{1}{3}\mathbf{I}\Big)\big(\mu_3(\sigma_{11}-\sigma_{33})+\mu_1(\sigma_{11}-\sigma_{22})\big)\\ &+\Big(\mathbf{n}_2\otimes\mathbf{n}_2-\frac{1}{3}\mathbf{I}\Big)\big(\mu_2(\sigma_{22}-\sigma_{33})+\mu_1(\sigma_{22}-\sigma_{11})\big)\\ &+\Big(\mathbf{n}_3\otimes\mathbf{n}_3-\frac{1}{3}\mathbf{I}\Big)\big(\mu_2(\sigma_{33}-\sigma_{22})+\mu_3(\sigma_{33}-\sigma_{11})\big)\\ &+6\mu_{12}\tau_{12}(\mathbf{n}_1\otimes\mathbf{n}_2+\mathbf{n}_2\otimes\mathbf{n}_1)+6\mu_{13}\tau_{13}(\mathbf{n}_1\otimes\mathbf{n}_3+\mathbf{n}_3\otimes\mathbf{n}_1)+6\mu_{23}\tau_{23}(\mathbf{n}_2\otimes\mathbf{n}_3+\mathbf{n}_3\otimes\mathbf{n}_2)\Big],\end{aligned}$$

with the expression for equivalent stress:

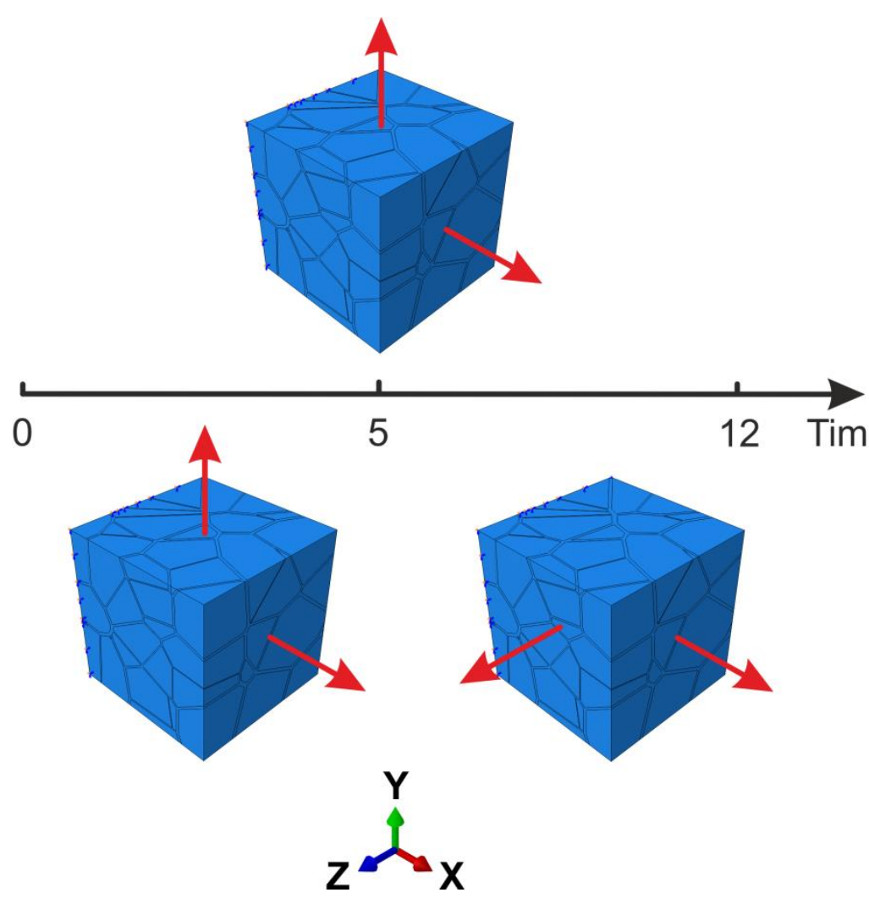
$$\sigma_{\mathrm{eq}}^2 \quad = \frac{1}{2}\mu_2(\sigma_{22}-\sigma_{33})^2+\frac{1}{2}\mu_3(\sigma_{33}-\sigma_{11})^2+\frac{1}{2}\mu_1(\sigma_{11}-\sigma_{22})^2+3\mu_{12}\tau_{12}^2+3\mu_{13}\tau_{13}^2+3\mu_{23}\tau_{23}^2.$$

- Creep material parameters for grain interior are taken from [3].
- Grain boundary region is used to simulate grain boundary sliding and reveals 'softer' creep behavior in comparison to grain interior. Due to this assumption the material parameter set for grain boundary region is obtained.
- The damage evolution law, based on the model of Tvergaard [4] is implemented for grain boundary region material in order to introduce creep cavitation. The change of creep strain rate due to cavitation is represented by means of (Cocks and Ashby [5]) formula.
- Stiffness reduction of the grain boundary region due to creep cavitation is considered.

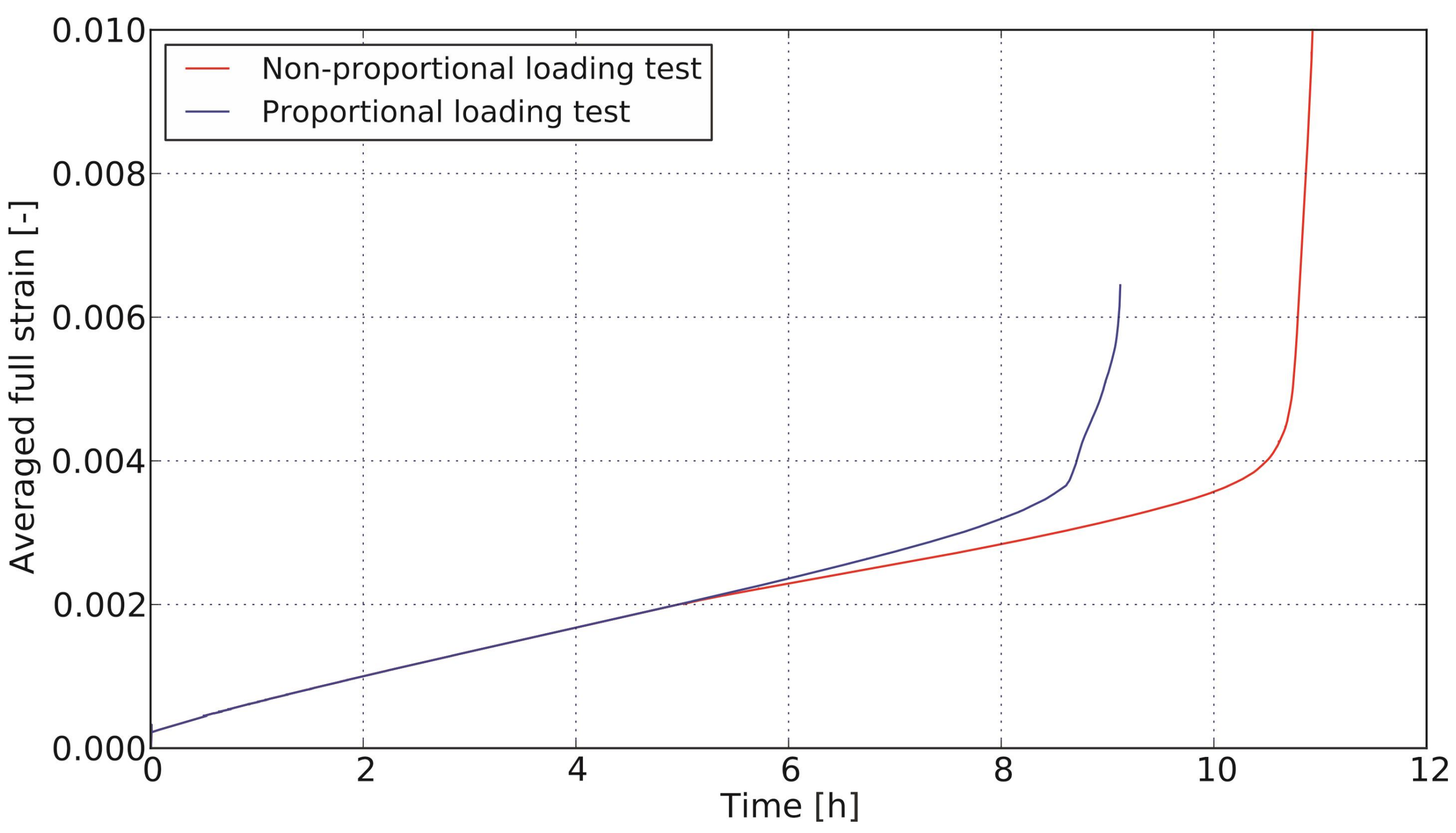
Model Application

Material parameter	**Grain interior**	**Grain boundary**
α_1^2, MPa	124700	360000
$\beta_1, \beta_2, \beta_3$, MPa	12333	12333
$\beta_{12}, \beta_{13}, \beta_{23}$, MPa	62300	62300
A, $(\mathrm{MPa})^{-n}/\mathrm{s}$	$1 \cdot 10^{-15}$	$6 \cdot 10^{-8}$
n	9.4	4
μ_1, μ_2, μ_3	1	0.2
$\mu_{12}, \mu_{13}, \mu_{23}$	0.2	0.3

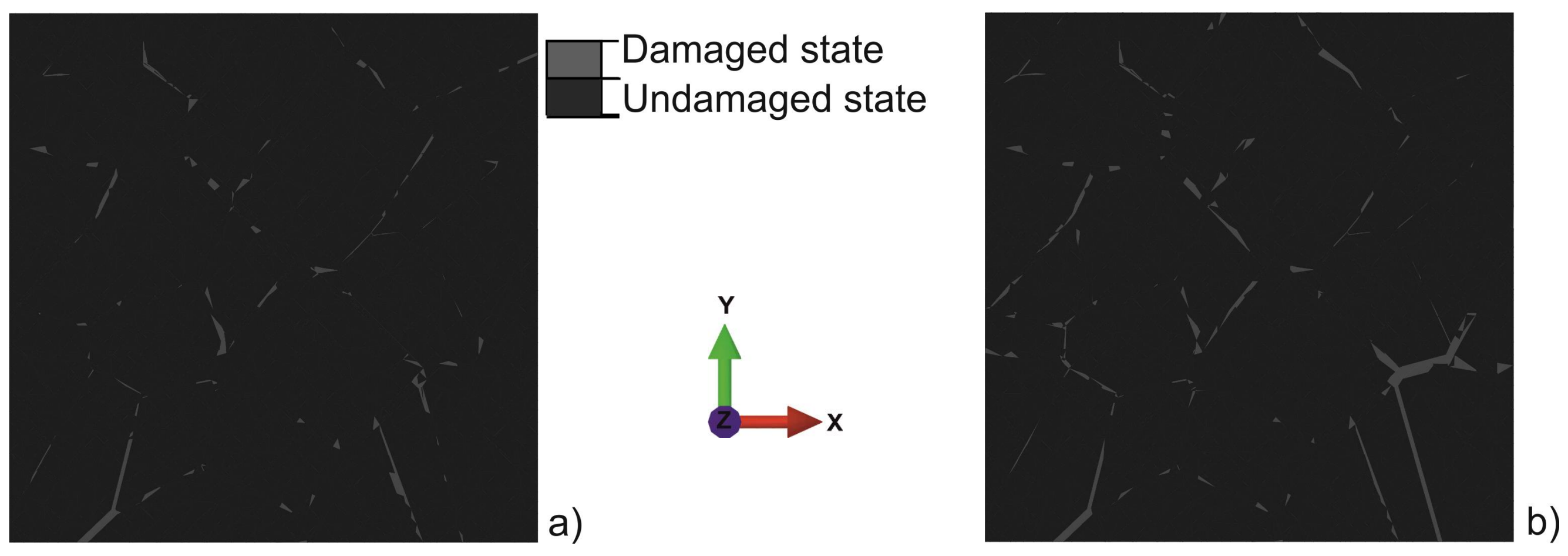
Material model parameters, taken for copper at 550 ˚C .



Scheme of the applied loading.



Evolution of the full strain in the *x*–direction with time for the case of proportional and non–proportional loading cases.



Distribution of damage in the cross–section of the unit cell after 9 hours of creep testing under a) non–proportional loading and b) proportional loading.

Results and Discussion

- Copper microstructure is simulated by means of a unit cell.
- Material model parameters are determined from elastic and creep tests of single crystal copper.
- Grain boundary sliding is validated by means of experimental data.
- Creep cavitation and stiffness reduction models are implemented to introduce the tertiary creep stage.
- The developed model is able to reflect phenomena observed during non-proportional loading tests:
  - For an averaged strain vs. time diagram strain rate decrease is detected after principal axes rotation;
  - Cross-section of the tested unit cell shows cavitation of grain boundaries orthogonal to the maximum principal stress ;
  - Prolongation of the time to rupture for the non-proportional loading case is observed. This can be explained by the fact, that after principal axes rotation other grain boundaries are involved in the cavitation process.

References:

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