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MESOSCOPIC APPROACH TO MODELING ELASTIC-PLASTIC POLYCRYSTALLINE MATERIAL BEHAVIOR

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ABSTRACT

Extreme loadings during severe accident conditions might cause failure or rupture of the pressure boundary of a reactor coolant system. Reliable estimation of the extreme deformations can be crucial to determine the consequences of such an accident. One of important drawbacks of classical continuum mechanics is idealization of inhomogenous microstructure of materials.

This paper discusses the mesoscopic approach to modeling the elastic-plastic behavior of a polycrystalline material. The main idea is to divide the continuum (e.g., polycrystalline aggregate) into a set of sub-continua (grains). The overall properties of the polycrystalline aggregate are therefore determined by the number of grains in the aggregate and properties of randomly shaped and oriented grains. The random grain structure is modeled with Voronoi tessellation and random orientations of crystal lattices are assumed. The elastic behavior of monocrystal grains is assumed to be anisotropic. Crystal plasticity is used to describe plastic response of monocrystal grains. Finite element method is used to obtain numerical solutions of strain and stress fields. The analysis is limited to two-dimensional models.

1 INTRODUCTION

Severe accidents in nuclear power plants are not included in the design basis events. Nevertheless, researchers worldwide are studying severe accident scenarios to predict their possible consequences. During severe accident conditions the pressure boundary of a reactor coolant system is subjected to extreme loading, which can cause failure or rupture. Reliable estimation of the extreme deformation of structural material can be crucial to determine the course of events and estimate the consequences of a severe accident.

Classical continuum mechanics cannot predict accurately the differences between measured responses of specimens, which are different in size but geometrical similar. The differences between expected material properties obtained by classical continuum mechanics and experimental data is defined as the size effect. A significant imperfection of classical continuum mechanics, which was not overcome even by the most complicated models (e.g., Gurson-Tvergaard damage mechanics model), is idealization of the inhomogenous microstructure of materials [1], [2].

Deformation of material can be, regarding the size, arranged in three regions with each having constitutive equations of their own: elastic, plastic (hardening) and damage regions

(softening). Classical continuum mechanics is suitable for describing elastic material behavior, but it relies on empirical models when plastic or damage behaviors are concerned. Empirical models can depend on large numbers of parameters, which can be hard to define, and demand experimental evaluation of each material and operational condition.

Classical continuum mechanics assumes homogeneity of material properties over the entire length scale and therefore independence of the length parameter. This is in contradiction with experimental data, which shows the importance of the length parameter in material behavior (size effect) [3].

Inhomogeneity of materials extends over the entire length scale, with each level having distinctive constitutive equations that describe material behavior on that level [4]. The constitutive equations of lower levels (e.g., micro- and mesoscopic) are usually simpler than macroscopic constitutive equations [5].

A computational model combining the most important mesoscale features and compatibility with conventional continuum mechanics is therefore sought. Room temperature is assumed to facilitate the comparison of numerical results with the results of simple tensile tests of a reactor pressure vessel steel [6].

2 MATERIAL MODEL

The main idea of the proposed approach is to divide the continuum (e.g., polycrystal aggregate) into a set of sub-continua (grains). The overall behavior of the aggregate is then sought through the combined response of the randomly shaped and oriented grains [7].

This requires the analysis to be carried out in two essential steps:

- Modeling of the random grain structure and
- Solution of underlying field equations.

The microstructure of the investigated pressure vessel steel (22 NiMoCr 3 7) is, at least in the broad sense, characterized as bainitic, based on α-Fe.

Currently available computational capabilities limit the analysis to a polycrystalline aggregate with a small number of grains and therefore also to 2-D.

The aim of the proposed approach is to cover:

- Elastic deformation and
- Rate-independent plastic deformation (low temperatures, to about 5-10% equivalent plastic strain).

The proposed approach has also a potential for generalization towards rate-dependent plasticity (creep) and initialization of microcracks at inclusions or voids.

2.1 Modeling of the Random Grain Structure

A Voronoi tessellation represents a cell structure constructed from a Poisson point process by introducing planar cell walls perpendicular to lines connecting neighboring points. This results in a set of convex polygons/polyhedra embedding the points and their domains of attraction, which completely fill up the underlying space.

The concept of Voronoi tessellation has recently been extensively used in materials science, especially to model random microstructures like aggregates of grains in polycrystals, patterns of intergranular cracks, and composites [8].

2.2 Strain/Stress Field in Crystal Grain

The basic idea of the elastic-plastic constitutive model is as follows:

- Each grain is assumed to be anisotropically elastic with random orientation of the crystal lattice.
- Plasticity model assumes plastic deformation by simple shear on the specified set of slip planes. The slip planes are essentially defined by orientation of the crystal lattice.

The material investigated is bainitic mild steel 22 NiMoCr 3 7. This implies body-centered cubic crystal with rather pronounced orthotropic elasticity. Each crystal grain is assumed to behave as a randomly oriented anisotropic continuum.

Constitutive relations in linear elasticity are given by the generalized *Hooke law* [1]:

$$\sigma_{ij} = C_{ijkl} \cdot \varepsilon_{kl}, \tag{1}$$

where σ_{ij} represents the stress tensor, C_{ijkl} the stiffness tensor, and ε_{ij} the strain tensor.

The elastic properties (e.g., stiffness and compliance tensor) of the polycrystalline aggregate are completely defined by the properties of, and interaction between, the crystal grains.

Within a grain it is assumed that plastic deformation takes place by simple shear on a specified set of slip planes. The plastic deformation rate $\dot{u}_{ij}^{p}$ due to crystallographic slip is given by [3]:

$$\dot{u}_{ij}^{p} = \sum_{\alpha} \dot{\gamma}^{(\alpha)} s_i^{(\alpha)} m_j^{(\alpha)}, \tag{2}$$

where $\dot{\gamma}^{(\alpha)}$ is the slipping rate, $s_i^{(\alpha)}$ the slip direction, and $m_j^{(\alpha)}$ the slip plane. Summation is performed over all slip systems α. With the assumption of small deformations, the plastic strain rate $\dot{\varepsilon}_{ij}^{p}$ can be written as:

$$\dot{\varepsilon}_{ij}^{p} = \sum_{\alpha} \frac{1}{2} \dot{\gamma}^{(\alpha)} \left(s_i^{(\alpha)} m_j^{(\alpha)} + s_j^{(\alpha)} m_i^{(\alpha)} \right). \tag{3}$$

The constitutive relation of the elastic-plastic crystal grain is now given, in terms of stress $\dot{\sigma}_{ij}$ and strain $\dot{\varepsilon}_{kl}$ rates, as:

$$\dot{\sigma}_{ij} = C_{ijkl} \cdot \left(\dot{\varepsilon}_{kl} - \dot{\varepsilon}_{kl}^{p} \right) = C_{ijkl} \cdot \dot{\varepsilon}_{kl} - C_{ijkl} \sum_{\alpha} \frac{1}{2} \dot{\gamma}^{(\alpha)} \left(s_i^{(\alpha)} m_j^{(\alpha)} + s_j^{(\alpha)} m_i^{(\alpha)} \right). \tag{4}$$

Equivalence of self- and latent hardening is assumed. Therefore, all slip systems are assumed to harden in an equivalent manner regardless of their activity.

The slipping rate $\dot{\gamma}^{(\alpha)}$ is frequently defined as the power law [9]:

$$\dot{\gamma}^{(\alpha)} = \dot{a}^{(\alpha)} \left(\frac{\tau^{(\alpha)}}{g^{(\alpha)}} \right) \left(\left| \frac{\tau^{(\alpha)}}{g^{(\alpha)}} \right| \right)^{n-1}, \tag{5}$$

where $\dot{a}^{(\alpha)}$ is reference strain rate, n the strain rate sensitivity parameter, $\tau^{(\alpha)}$ the shear stress, and $g^{(\alpha)}$ the current strain hardened state of the crystal derived from:

$$\dot{g}^{(\alpha)} = \sum_{\beta} h_{\alpha\beta} \dot{\gamma}^{(\beta)}, \tag{6}$$

where $h_{\alpha\beta}$ are the slip hardening moduli.

The simple form for the self-hardening moduli is given by [9]:

$$h_{\alpha\alpha} = h(\gamma) = h_0 \operatorname{sech}^2 \left| \frac{h_0 \gamma}{\tau_S - \tau_0} \right|, \tag{7}$$

where h_0 is the initial hardening modulus, τ_0 the yield stress, which equals the initial value of current strength $g^{(\alpha)}(0)$, τ_S the break-through stress where large plastic flow initiates, and γ the cumulative slip on all slip systems integrated by time t:

$$\gamma = \sum_{\alpha} \int_0^t \left| \dot{\gamma}^{(\alpha)} \right| dt \,. \tag{8}$$

The latent hardening moduli are given by:

$$h_{\alpha\beta} = q \cdot h(\gamma) \,. \tag{9}$$

where q is hardening factor.

A constitutive assumption that is often a reasonable approximation at ordinary temperatures, strain rates and pressures, is that the slipping rate $\dot{\gamma}^{(\alpha)}$ depends on the stress only through the Schmid resolved shear stress $\tau^{(\alpha)}$:

$$\tau^{(\alpha)} = s_i^{(\alpha)} \sigma_{ij} m_i^{(\alpha)} \,. \tag{10}$$

2.2.1 Material Parameters

Some of the material parameters are obtained from results of a simple tensile test of 5 mm specimen made of pressure vessel steel (22 NiMoCr 3 7) [6]. Since no tensile tests were made on monocrystals for this material, missing parameters are obtained from the literature for α-Fe [10]. It is assumed that small amounts of alloying elements do not change the elastic stiffness/compliance of a crystal grain significantly.

The components of the stiffness tensor are c_{11} = 230 GPa, c_{12} = 130 GPa, and c_{44} = 117 GPa [11]. Hardening (macroscopic) parameters obtained from the results of simple tensile test [6] are: initial yield stress τ_0 = 450 MPa, stage I stress τ_S = 45 MPa, and initial hardening modulus h_0 = 658 MPa.

A straightforward way to derive the parameters of the monocrystal hardening from the macroscopic behavior is given in [12]. The microscopic parameters are defined by:

$$\tau_{0\,micro} = \frac{\tau_{0\,macro}}{M}, \quad \tau_{S\,micro} = \frac{\tau_{S\,macro}}{M} \quad \text{and} \quad h_{0\,micro} = \frac{h_{0\,macro}}{M^2}, \tag{11}$$

where M is the Taylor factor. Therefore microscopic values are: for initial yield stress $\tau_{0\ micro}$ = 155 MPa, stage I stress $\tau_{S\ micro}$ = 15.5 MPa, and initial hardening modulus $h_{0\ micro}$ = 70 MPa. Reference strain rate $\dot{a}$ = 0.001 and rate sensitivity exponent n = 50. Taylor hardening is used, therefore q = 1 [9].

3 PRELIMINARY RESULTS

To illustrate this mesoscopic approach to modeling the elastic-plastic behavior of a polycrystalline aggregate with 11 grains is used. This represents a specimen with dimensions 100 μm × 70 μm. Analysis was limited to 11 grains due to the limitations in currently available computational capabilities.

The finite element model of the 11-grain aggregate is shown in Figure 1. The grain boundaries are plotted in red. The blue lines are introduced exclusively to facilitate mesh generation. The crystal lattice orientation of each grain is plotted with black arrows. The polycrystalline aggregate was loaded monotonically by increasing the remote stress in the *x*-direction (up to $\sigma_{x\,max}$ = 1000 MPa).

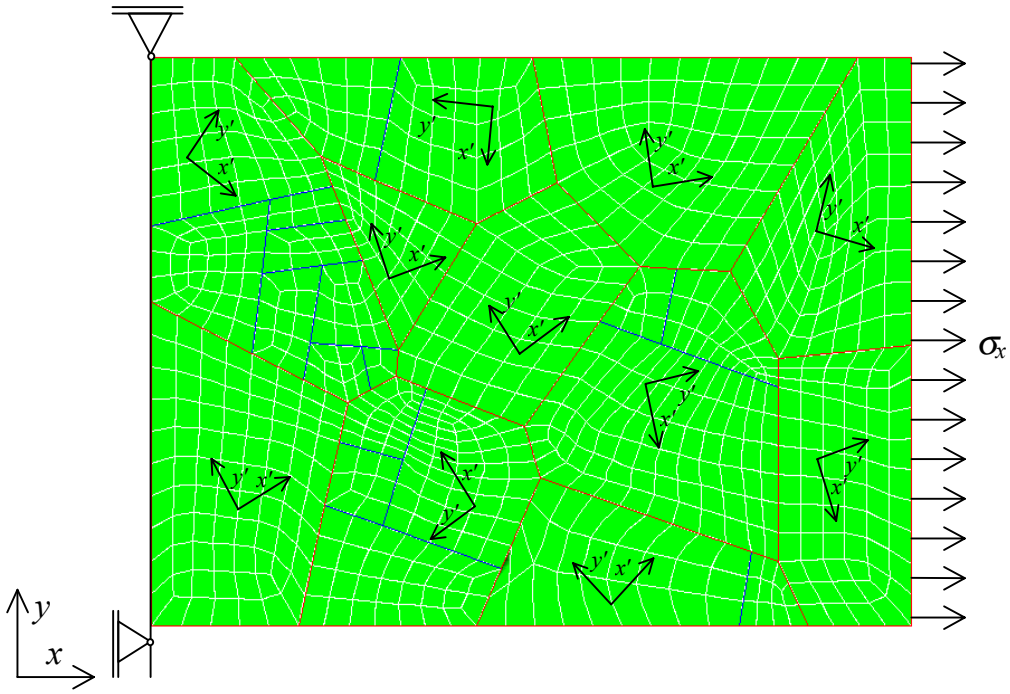

Figure 1 **Finite element model of a polycrystal with 11 grains (black arrows show crystal lattice orientation of each grain, red lines are grain boundaries, blue lines are introduced to facilitate the meshing)**

Anisotropic elastic behavior and random orientations of grains was assumed. Crystal plasticity model is used to describe plastic behavior.

The selection of boundary conditions has a large influence on the results [3], [13]. The stress boundary conditions can cause too weak a behavior of the grains and displacement boundary conditions too stiff a response. For illustrative purposes only the case with stress boundary conditions was taken into account.

General-purpose finite element code ABAQUS [14] was used for numerical calculations. For application of the crystal plasticity model a user material subroutine [9] was used.

3.1 Stress/Strain Relations

Some preliminary results of the simulation in the form of uniaxial true stress/true strain diagrams are shown in Figure 4. True stresses and strains in the *x*-direction are used. True

strain is obtained by averaging true strains on the boundary of the polycrystalline aggregate as shown in Figure 2. Uniaxial stresses are used here to enable comparison between numerical results and results of tensile tests.

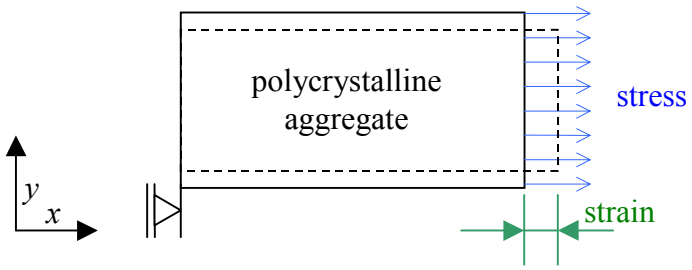

Figure 2 Obtaining strains and stresses from numerical simulation

The results of polycrystalline aggregate are compared with results of two simple monocrystal models. The difference in monocrystal models is in orientation of crystal cells within the crystal as depicted in Figure 3.

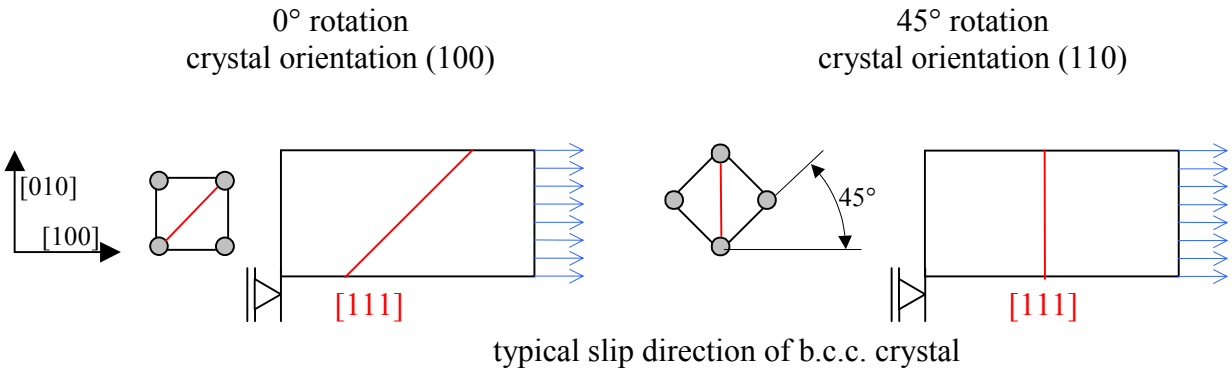

Figure 3 Typical slip directions of b.c.c. crystal due to the rotation of the crystal lattice

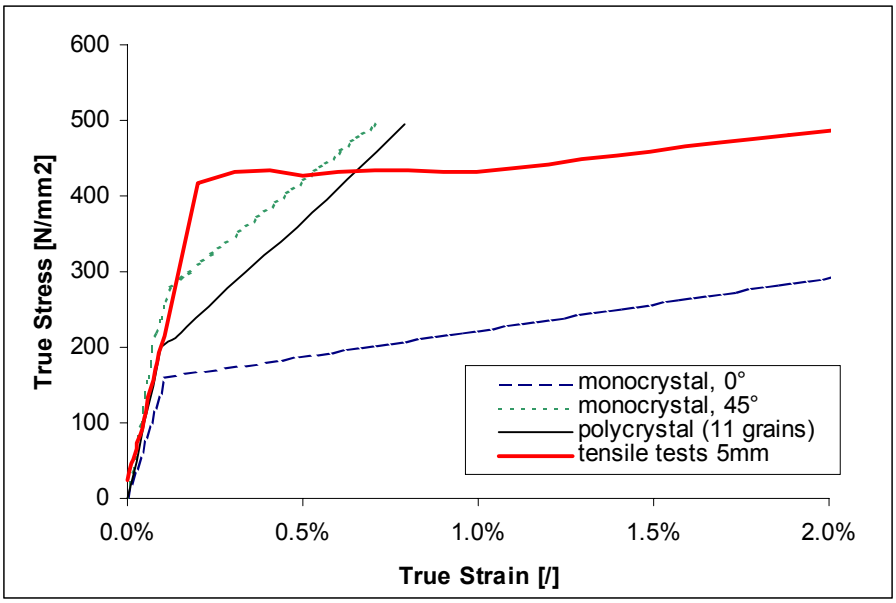

Figure 4 Results of numerical simulations of single and polycrystal and results of tensile tests

The elastic properties obtained by numerical simulation of polycrystalline aggregate are in accordance with results of the tensile tests. The results of plastic responses show large discrepancies. Numerically obtained yield strength is only about 40% of the yield strength achieved by tensile tests (yield strength was obtained as true stress at 0.2% true strain). These discrepancies are mainly due to the size of polycrystalline aggregate used in numerical simulation (11 grains, size approximately 100 μm × 70 μm). This is significantly smaller than the representative volume element for metals as described in the literature (e.g., [3]). A larger polycrystalline aggregate (with more crystal grains) should be used to obtain more accurate results. Use of 3D-polycrystalline aggregate would probably also improve the accuracy of the results.

Influence of weak behavior of the grains caused by boundary conditions, which are imposed on polycrystalline aggregate, is considered, due to small number of grains [13], smaller than the influence of the size and thus cannot be observed.

The difference between responses of two monocrystals is due to the rotation of the crystal lattice. Slip in slip systems mainly depends on shear stress. Typical slip direction in b.c.c. crystal is [111], which in non-rotated crystal lattice corresponds with the direction of maximum shear stresses (see Figure 3a). This means less stress is needed for slip systems to slide than in crystal, which has the crystal lattice rotated by 45° (see Figure 3b).

3.2 Stress/Strain Fields

Figures 5 and 6 show the results for the polycrystalline aggregate subjected to uniaxial loading. The grain boundaries are plotted in white. The differences in stresses during the slip along the slip planes are shown.

Figure **5** shows the shear stress, which is responsible for yielding The shear direction is oriented randomly (in accordance with orientation of the crystal lattice of each grain as shown on Figure 1), which results in very pronounced differences between grains.

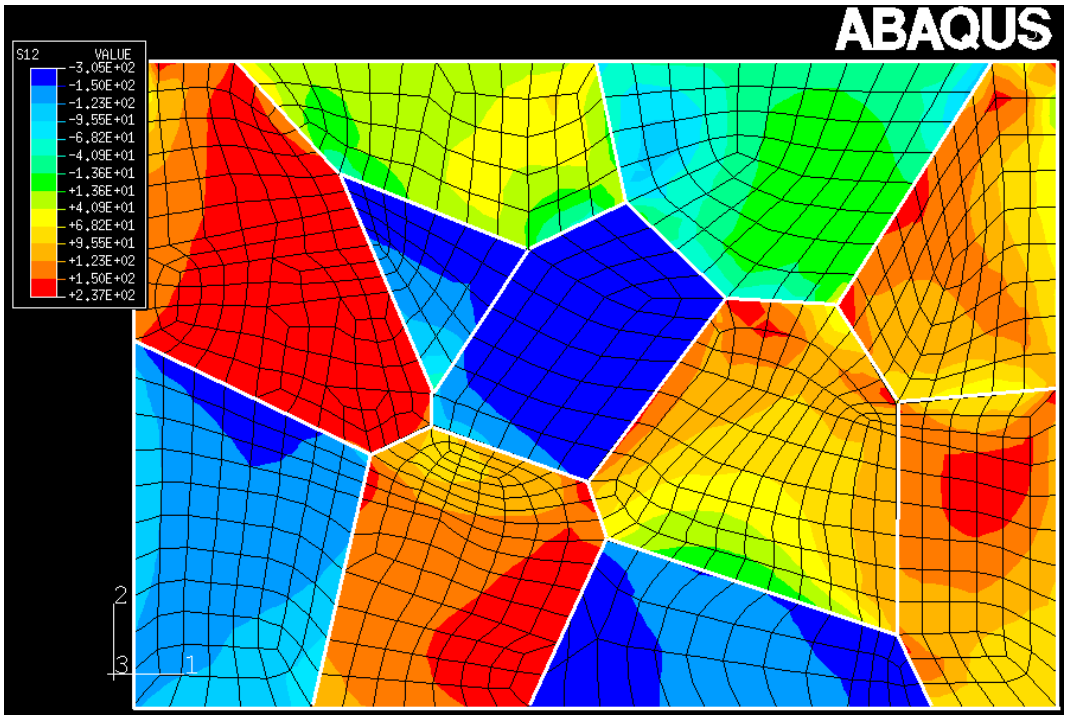

Figure 5 Shear stress (in local directions)

Figure 6 shows von Mises equivalent stress. The regions with concentrations are clearly shown. The difference in the results is in the order of • 20%. The higher stresses in the middle of the specimen are due to the orientations of the crystal lattices within grains and not to the occurrence of shear banding. Concentration at the triple points may originate from numerical approximations and simplifications.

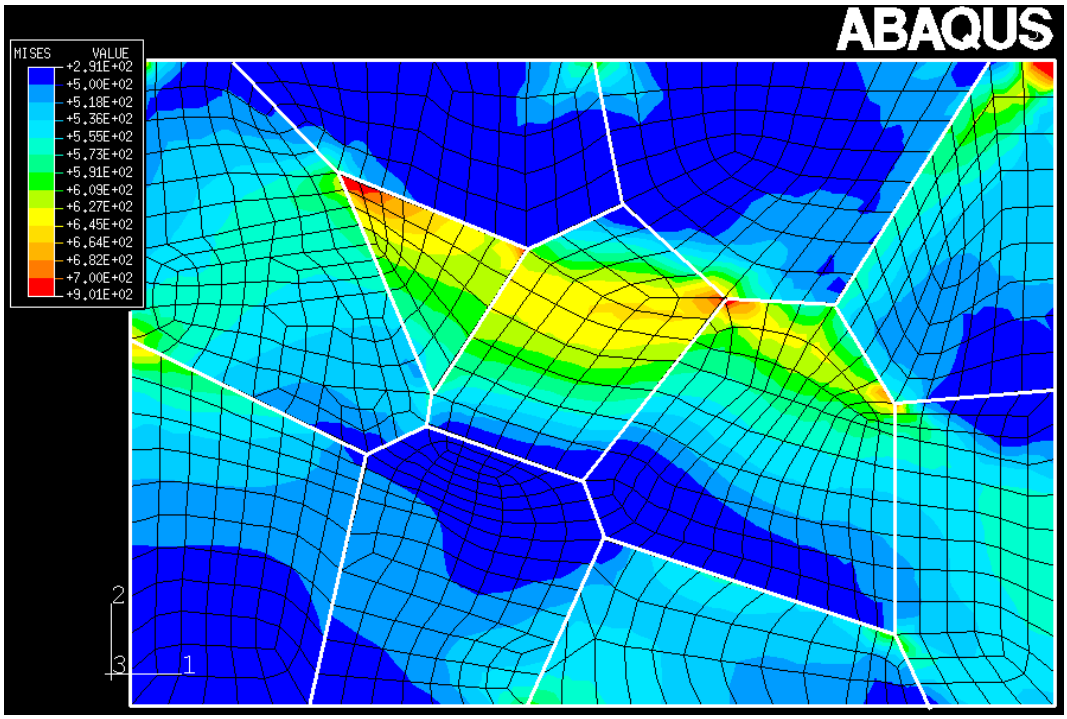

Figure 6 Equivalent stress (von Mises)

4 CONCLUSIONS

Extreme loadings during severe accident might cause failure of the pressure boundary of reactor coolant system. Reliable estimation of the extreme deformations is therefore essential to determine the consequences of such a severe accident.

The proposed mesoscopic approach to modeling elastic-plastic polycrystalline material behavior is based on two essential components:

- Modeling of the geometrical aspects of random grain structure using Voronoi tessellation. Each of the grains has random orientation.
- Solution of underlying field equation. Finite element method is used.

The proposed approach covers elastic deformation and rate independent plastic deformation. The agreement between elastic properties obtained by numerical simulation of polycrystalline aggregate and results of the tensile test is satisfactory. However, the results of plastic responses show large discrepancies between numerical simulation and test results. This is mainly due to a small size of polycrystalline aggregate used in numerical simulation.

Polycrystalline aggregates with larger number of grains are expected to be used in the future. They are expected to reduce the discrepancies between numerical solutions and results of tensile tests. Sensitivity analysis regarding number of grains of aggregate, grain orientation, number of finite element within grains (mesh density) and effect of boundary conditions will also be performed.

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