ESTIMATING MINIMUM POLYCRYSTALLINE AGGREGATE SIZE FOR MACROSCOPIC MATERIAL HOMOGENEITY

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ABSTRACT

During severe accidents the pressure boundary of reactor coolant system can be subjected to extreme loadings, which might cause failure. Reliable estimation of the extreme deformations can be crucial to determine the consequences of severe accidents. Important drawback of classical continuum mechanics is idealization of inhomogenous microstructure of materials. Classical continuum mechanics therefore cannot predict accurately the differences between measured responses of specimens, which are different in size but geometrical similar (size effect). A numerical approach, which models elastic-plastic behavior on mesoscopic level, is proposed to estimate minimum size of polycrystalline aggregate above which it can be considered macroscopically homogeneous. The main idea is to divide continuum into a set of sub-continua. Analysis of macroscopic element is divided into modeling the random grain structure (using Voronoi tessellation and random orientation of crystal lattice) and calculation of strain/stress field. Finite element method is used to obtain numerical solutions of strain and stress fields. The analysis is limited to 2D models.

1   INTRODUCTION

During severe accidents the pressure boundary of reactor coolant system can be subjected to extreme loadings, which might cause failure. Reliable estimation of the extreme deformations of material (steel) can be crucial to determine the course of events and estimate the consequences of severe accidents. Therefore a lot of efforts were made during past few years to determine mechanical properties of polycrystalline aggregates of different sizes.

Important drawback of classical continuum mechanics, which was not overcome by the existing models (e.g., Gurson-Tvergaard damage mechanics model), is idealization of inhomogenous microstructure of materials [1], [2]. Classical continuum mechanics therefore 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.

As a result some approaches appeared for modeling of material on mesoscopic levels with emphasis on predictions of the behavior of polycrystalline aggregates with consideration of material microstructure [2]. Approaches, which use stochastic methods to represent microstructure of material and anisotropic material model, were introduced only recently [2], [3].

The main goal of the paper is to propose an approach, which models elastic-plastic behavior on mesoscopic level, to estimate minimum size of polycrystalline aggregate above which it can be considered macroscopically homogeneous. The estimation of minimal size of mesoscopically inhomogenous, but macroscopically homogenous, material is based on comparing macroscopic quantities of polycrystalline aggregates.

The main idea of proposed mesoscopic approach is to divide continuum (e.g., polycrystalline aggregate) into a set of sub-continua (grains). Overall properties of the polycrystalline aggregate are outcome of number of grains in the aggregate and properties of randomly shaped and oriented grains. Analysis of macroscopic element is divided into modeling the random grain structure (using Voronoi tessellation and random orientation of crystal lattice) and calculation of strain/stress field. Mesoscopic response of monocrystal grains is modeled with anisotropic elasticity and crystal plasticity.

Finite element method, which proved as suitable [2], is used to obtain numerical solutions of strain and stress fields. The analysis is limited to two-dimensional models. Material parameters for pressure vessel steel 22 NiMoCr 3 7 with bainitic microstructure with b.c.c. crystals are used in analysis.

2 MATERIAL MODEL

Basic assumptions of material model are:
- Random polycrystalline structure is represented by a Voronoi tessellation.
- Each grain is assumed to be a monocrystal with random orientation of crystal lattice. Anisotropic elastic behavior of grains is assumed.
- A model of plasticity assumes that plastic deformation is caused by crystalline slip on predefined slip planes of crystal lattice. Slip planes and direction are defined by orientation of crystal lattice, which differs from grain to grain (random orientation).

2.1 Voronoi tessellation

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 [4], [5], [6]. 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 (Figure 1) embedding the points and their domains of attraction, which completely fill up the underlying space. All Voronoi tessellations used for the purpose of this paper were generated by the code VorTess [7].
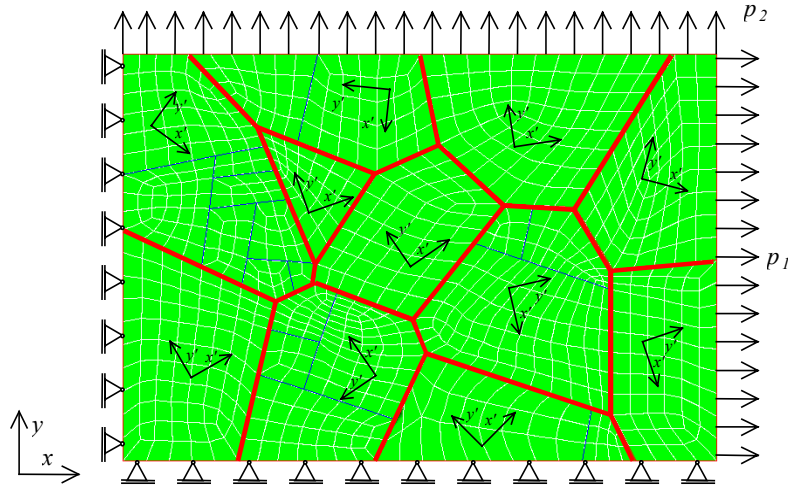
Figure 1: Voronoi tessellation with highlighted grain boundaries, orientations of crystal lattices and finite element mesh

2.2 Anisotropic Elasticity

Pressure vessel steel 22 NiMoCr 3 7 has body-centered cubic crystal lattice with rather pronounced orthotropic elasticity. Each crystal grain is assumed to behave as a randomly oriented anisotropic continuum. Constitutive relations are given by the generalized Hooke's law [8]:

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

where σ_{ij} represents the stress tensor, C_{ijkl} the stiffness tensor, and ε_{kl} 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. Material parameters for elasticity are obtained from the literature for α-Fe for body-centered cubic crystal lattice (e.g., [9], [10]). It is assumed that small amounts of alloying elements do not change the elastic stiffness/compliance of a crystal grain significantly [10]. The nonzero components of the stiffness tensor are $c_{iiii} = 230$ GPa, $c_{iijj} = 135$ GPa and $c_{ijij} = 117$ GPa [10].

2.3 Crystal Plasticity

Assumtion of crystal plasticity is that plastic deformation is a result of crystalline slip only. It is assumed that crystalline slip is driven by resolved shear stress $\tau^{(\alpha)}$ [11]:

$$\tau^{(\alpha)} = m_i^{(\alpha)} \cdot \sigma_{ij} \cdot s_j^{(\alpha)},$$
(2)

where α-th slip system is defined by a combination of slip plane (determined by normal $m_i^{(\alpha)}$) and slip direction ($s_j^{(\alpha)}$) of crystal lattice. Body-centered cubic crystal lattice has three families of slip planes: {110}, {112}, and {123} and one family of slip directions: <111>. This leads to 48 possible slip systems [8]. Stress rate can be defined as:

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

Rate-independent plasticity may be treated as the limit of the rate-dependent visco-plasticity [11]. The slipping rate $\dot{\gamma}^{(\alpha)}$ of the α-th slip system is determined by the corresponding resolved shear stress $\tau^{(\alpha)}$ as:

$$\dot{\gamma}^{(\alpha)} = \dot{a}^{(\alpha)} \left(\frac{\tau^{(\alpha)}}{g^{(\alpha)}} \right) \left(\left| \frac{\tau^{(\alpha)}}{g^{(\alpha)}} \right| \right)^{n-1}, \tag{4}$$

where $a^{\cdot(\alpha)}$ is reference strain rate, n the strain rate sensitivity parameter and $g^{(\alpha)}$ the current strain hardened state of the crystal. In the limit as n approaches infinity this power law approaches that of a rate-independent material.

The current strain hardened state $g^{(\alpha)}$ can be derived from:

$$\dot{g}^{(\alpha)} = \sum_{\beta} h_{\alpha\beta} \dot{\gamma}^{(\beta)}, \tag{5}$$

where $h_{\alpha\beta}$ are the slip hardening moduli. More authors dealt with hardening moduli (e.g., [11], [12]), with all of them basing their work on empirical models. Pierce et. al. and Asaro [12] hardening law is used in our research. Self- (index $_{\alpha\beta}$) and latent-hardening moduli ($_{\alpha\alpha}$) are defined as:

$$h_{\alpha\alpha} = h(\gamma) = h_0 \, \mathrm{sech}^2 \left| \frac{h_0 \gamma}{\tau_S - \tau_0} \right| \text{ and } h_{\alpha\beta} = q h(\gamma), \; (\alpha \neq \beta), \tag{6}$$

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, γ the cumulative slip and q is hardening factor.

Material parameters for plasticity are obtained from literature for rate-independent crystal plasticity (e.g., [8]) and from results of simple tensile test of pressure vessel steel 22 NiMoCr 3 7 [13]. The following values were used: the strain rate sensitivity parameter $n = 50$, the reference strain rate $\dot{a}^{(\alpha)} = 0.001$ s^{-1}, the initial hardening modulus $h_0 = 70$ MPa, the break-through stress $\tau_S = 15.5$ MPa, yield stress $\tau_0 = 155$ MPa and hardening factor $q = 1$.

Equations (3)-(6), which describe rate-dependent elasto-plastic deformations of crystals, are given in incremental form for use with finite element method [11]. Large number of slip systems (48 for b.c.c. crystals) causes conventional time-integration scheme to become exceedingly inefficient [8]. This leads to a very small incremental step and long computational time needed to ensure solution stability. Therefore only analyses with models with up to 110 grains (212 in elasticity) were carried out at this time.

2.4 Estimation of Representative Volume Element Size

Minimal size of mesoscopically inhomogenous material, but macroscopically homogenous, is usually called representative volume element (RVE). At volumes of mesoscopically inhomogenous material larger than RVE size effect on macroscopic level cannot be observed [8]. Macroscopic quantities are averaged over all polycrystalline aggregate. A condition when RVE size is achieved is defined as [14]:

$$C^*_{ijkl} \cong \left(D^*_{ijkl} \right)^{-1}, \tag{7}$$

where C^*_{ijkl} and D^*_{ijkl} are macroscopic stiffness and compliance tensors (for polycrystalline aggregate) [14]. This sets the bounds below which proposed mesoscopical approach is more suitable to model the elastic-plastic response of material.

Equation (7) is in general not valid for polycrystalline aggregates smaller than RVE. The different behavior of both tensors is governed by the size of the aggregate and macroscopic boundary conditions [11]: macroscopic stiffness tensor therefore assumes stress driven boundary condition, while macroscopic compliance tensor assumes displacement

driven boundary condition. With general relations between stresses and strains in mind (as for instance described in equation (1)), equation (7) can be simplified by using macroscopic equivalent stresses $<\sigma_{eq}>$:

$$\left\langle \sigma_{eq\,s} \right\rangle \cong \left\langle \sigma_{eq\,d} \right\rangle, \tag{8}$$

where indexes $_s$ and $_d$ denote stress and displacement driven boundary conditions, respectively. This simplified condition is sufficient to present the crucial trends [5]. Some authors (e.g., [15]) have used an extrapolation to estimate RVE size. The extrapolation is based on size of polycrystalline aggregate, which is smaller than RVE size. Relation between stiffness and compliance tensors for that polycrystalline aggregate can be written as [15]:

$$C^*_{ijkl} \cdot D^*_{klmn} = I_{ijmn} + O(V/V_{RVE}), \tag{9}$$

where V_{RVE} represents RVE size, V size of polycrystalline aggregate smaller than RVE, I_{ijmn} 4-th rank unit tensor and O estimate of residuum. With equation (8) and proportionality between number of grains in polycrystalline aggregate and its size in mind, one can use:

$$\frac{\left\langle \sigma_{eq\,s} \right\rangle}{\left\langle \sigma_{eq\,d} \right\rangle} = 1 + O(i/i_{RVE}), \tag{10}$$

where i_{RVE} represents number of grains in RVE and i number of grains size in polycrystalline aggregate smaller than RVE. A RVE is achieved, when residuum O is smaller than 1% [15].

3   RESULTS

Results of the proposed numerical approach are presented in this section. Examples of macroscopic response of polycrystalline aggregates with different orientation of crystal lattice are shown.

3.1   Strain/stress Curves

Figure 2 shows a relationship between macroscopic equivalent (Von Mises) stress and macroscopic equivalent strain for 30 cases with different orientations of crystal lattice for 14-grain polycrystalline aggregate with displacement and stress boundary conditions.
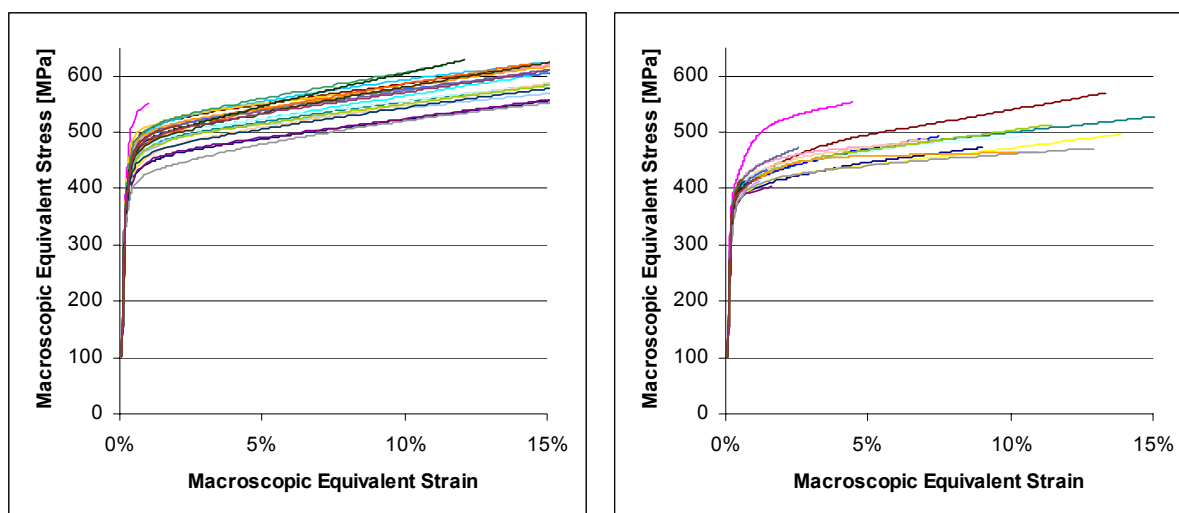
Figure 2: A relationship between macroscopic equivalent stress and macroscopic equivalent strain with displacement (left) and stress driven boundary conditions (right)

A scatter of curves due to different orientations of crystal lattice within plasticity is clearly visible. Nevertheless curves within elasticity nearly coincide, but with quite distinctive scatter of yield points. Stress boundary condition in average causes conventional time-integration schemes to be even more inefficient. This leads to fewer different randomly oriented crystal lattices with stress boundary condition to be analyzed (without severe decrease of incremental steps).

3.2   Estimation of RVE Size within Elasticity

Analyses in elasticity were carried out on models with 14, 23, 53, 110 and 212 grains. 30 different random orientations of crystal lattices and 2 boundary conditions (stress and displacement boundary conditions) were analyzed for each model. Analyses were carried out at macroscopic stress p_{11} = 200 MPa and p_{22} = 100 MPa (Figure 1). Results were compared with an analytical solution for macroscopically homogenous material obtained by continuum elasticity model with material parameters: E = 210 GPa and ν = 0.29 [4]. Results are shown in Figure 3 (left), where d in the legend refers to displacement boundary condition, s refers to stress boundary condition and *ave* refers to average values (averaged over 30 different randomly oriented crystal lattices with displacement or stress boundary conditions). The number following abbreviation denotes number of grains of polycrystalline aggregates. Analytical solution (classical continuum mechanics) for macroscopic homogenous material ($<\varepsilon_{eq}>$ = 0.0515% and $<\sigma_{eq}>$ = 96.2 MPa) is also shown.

A tendency towards decrease of scatter of results as number of grains in the models increases can be observed. Average values of stresses and strains (for both boundary conditions) show a clear trend towards analytical solution with increasing number of grains in the model. With residuum for 212-grain aggregate (equation(10)) over 1%, one can conclude that RVE has not been achieved.
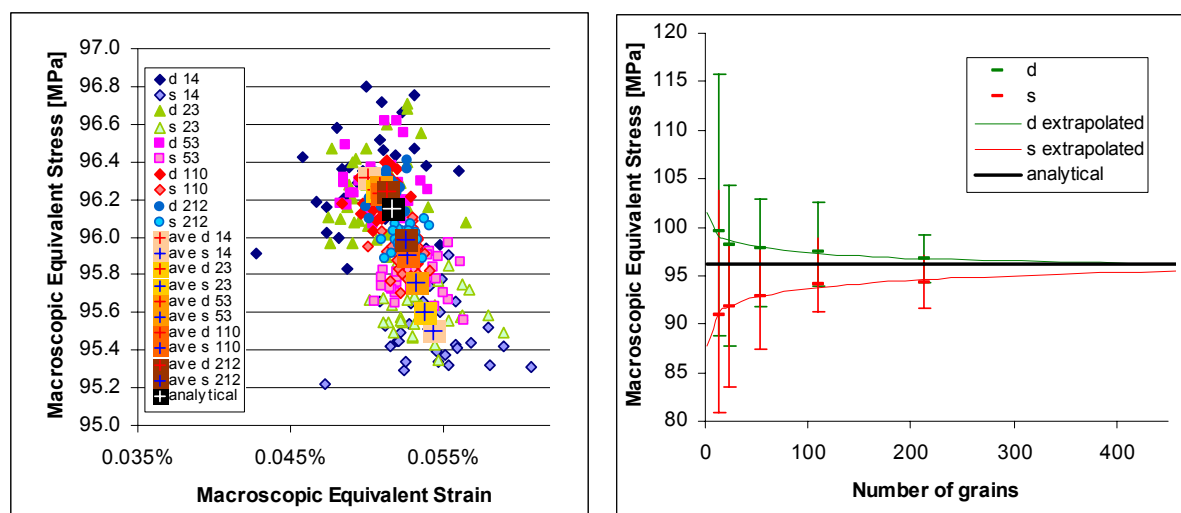
Figure 3: Scatter of macroscopic equivalent strain/stress (left) and convergence of macroscopic equivalent stresses in elasticity (right)

To estimate RVE size in elasticity, macroscopic equivalent stresses were taken at macroscopic equivalent strain of $<\varepsilon_{eq}>$ = 0.0515 % (in accordance with the analytical solution). Figure 3 (right) shows macroscopic equivalent stresses and scatter depending on number of grains in polycrystalline aggregate for displacement (denoted as *d*) and stress (denoted as *s*) driven boundary conditions. Extrapolation lines are drawn in accordance with equation (9).

Trend toward analytical solution and decrease of scatter with increasing number of grains is again clearly visible. Preliminary RVE size is estimated from equation (9). Based on equation (10), the preliminary estimation of RVE size is 280 grains, which corresponds to a polycrystalline aggregate of about 0.3 mm in size. Although these results are only estimations, one can nevertheless conclude that results are within expected from literature (e.g., [15]).

3.3 Estimation of RVE Size within Plasticity

Analyses in plasticity were carried out on models with 14, 23, 53, and 110 grains. 30 different random orientations of crystal lattices and 2 boundary conditions (stress and displacement boundary conditions) were analyzed for each model. Analysis was performed at macroscopic stress p_{11} = 1000 MPa and p_{22} = 500 MPa (Figure 1).

Very small incremental step is needed to ensure solution stability due to inefficiency of conventional time-integration scheme [8]. Hence, long computational time is necessary to obtain reasonable solution. A small initial step of 1% of total stress scale was used in plasticity, which nevertheless leaded to premature end of some analyses. Even smaller time step or unconventional time-integration schemes (e.g., [8]) should be used in the future. At this stage, the above-mentioned numerical difficulties did not allow for all 30 different randomly oriented crystal lattices to be analyzed. Nevertheless, the available results enable us to show and explain the essential tendencies.

Average values of macroscopic equivalent stresses and strains were calculated over all different randomly oriented crystal lattices for each model and boundary condition. Results are shown in Figure 4 (left), where *d* in the legend refers to displacement boundary condition, *s* refers to stress boundary condition and *ave* refers to average values (for displacement and stress boundary conditions). The number following abbreviation denotes number of grains of polycrystalline aggregates. A tendency towards decrease of scatter of results with increasing number of grains in the models can be observed. Average values of stresses and strains (for both boundary conditions) show a clear trend towards a common average value with

increasing number of grains in the model. Residuum (equation (10)) with 110-grain aggregate is around 5% therefore one can conclude that RVE has not been achieved.
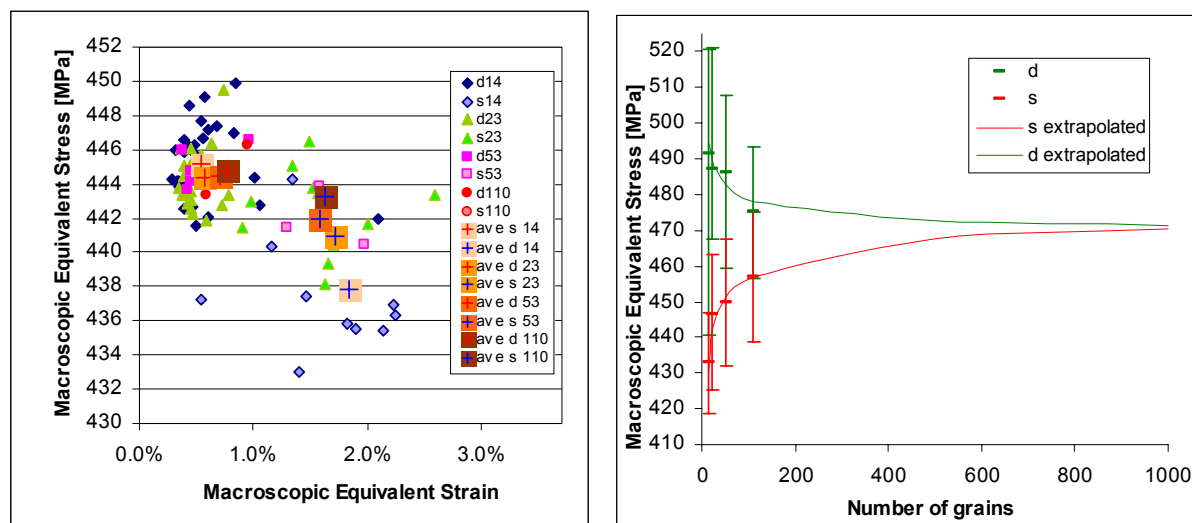
Figure 4: Scatter of macroscopic equivalent strain/stress (left) and convergence of macroscopic equivalent stresses in plasticity (right)

The same approach to estimate preliminary RVE size as in elasticity was used. Macroscopic equivalent stresses were taken at macroscopic equivalent strain of $<\varepsilon_{eq}> = 1\%$. Figure 4 (right) shows macroscopic equivalent stresses and scatter depending on number of grains in polycrystalline aggregate for displacement (denoted as d) and stress (denoted as s) driven boundary conditions. Extrapolation lines are drawn in accordance with equation (9).

A tendency toward a common average value and smaller scatter is visible. Preliminary estimation of RVE size is 750 grains, which corresponds to a polycrystalline aggregate of 0.6 mm in size, with residuum (equation (10)) of 1%.

4 SUMMARY

A numerical approach, which models elastic-plastic behavior on mesoscopic level, was proposed to estimate minimum size of polycrystalline aggregate above which it can be considered macroscopically homogeneous. An estimation of minimal size of mesoscopically inhomogenous, but macroscopically homogenous, material is crucial to estimate limits of classical continuum mechanics. An approach combines the most important mesoscale features and compatibility with conventional continuum mechanics to model elastic-plastic behavior. Explicit modeling of the random grain structure is used. Grains are regarded as monocrystals (modeled with anisotropic elasticity and crystal plasticity).

Proposed approach enables estimation of minimum size of polycrystalline aggregate above which it can be considered macroscopically homogeneous. The RVE size above which polycrystalline aggregate can be considered macroscopic homogeneous within elasticity is estimated to 280 grains, which corresponds to a specimen of about 0.3 mm in size. The RVE size within plasticity is estimated to 750 grains, which corresponds to a specimen of about 0.6 mm in size. The RVE sizes set the bounds below which proposed mesoscopical approach is more suitable to model the elastic-plastic response of material.

Finalization of RVE estimates in elasticity and plasticity is foreseen in the near future. This will include integration of non conventional time-integration scheme.

5 REFERENCES

[1] Needleman, A. Computational Mechanics at the Mesoscale. Acta Materialia. 2000; 48:105-124.

[2] Watanabe, Osamu; Zbib, Hussein M., and Takenouchi, Eiji. Crystal Plasticity, Micro-shear Banding in Polycrystals using Voronoi Tessellation. International Journal of Plasticity. 1998; 14(8):771-778.

[3] Kovač, Marko and Cizelj, Leon. Mesoscopic Approach to Modeling Elastic-Plastic Polycrystalline Material Behavior. Proc of Int Conf Nuclear Eergy in New Europe 2001; Portorož, Slovenia. 2001.

[4] Cizelj, Leon and Kovač, Marko. Constitutive Models for the Elastic-Plastic Polycrystalline Aggregate with Stohastic Arrangement of Grains. Rev 0. Ljubljana: Institut Jožef Stefan; 2001; IJS-DP-8334.

[5] Cizelj, Leon; Kovač, Marko; Petrič, Zoran; Fabjan, Ljubo, and Mavko, Borut. Efects of Grain Structure on Elastic-plastic Behavior of Polycrystalline Aggregate. Ljubljana: Institut Jožef Stefan; 2002; IJS-DP-8547.

[6] Aurenhammer, Franz. Voronoi Diagrams-A Survey of a Fundamental Geometric Data Structure. ACM Computing Surveys. 1991; 23(3):345-405.

[7] Riesch-Oppermann, Heinz. VorTess, Generation of 2-D random Poisson-Voronoi Mosaics as Framework for the Micromechanical Modelling of Polycristalline Materials. Karlsruhe, Germany: Forschungszentrum Karlsruhe; 1999; Report FZKA 6325.

[8] Nemat-Nasser, Sia; Okinaka, Tomoo, and Ni, Luqun. A Physically-based Constitutive Model for BCC Crystals with Application to Polycrystalline Tantalum. Journal of the Mechanics and Physics of Solids. 1998; 46(6):1009-1038.

[9] Nye, J. F. Physical Properties of Crystals. Oxford: Clarendon Press; 1985.

[10] Grimvall, Göran. Thermophysical Properties of Materials. Amsterdam: North-Holland; 1999.

[11] Huang, Yonggang. A User-material Subroutine Incorporating Single Crystal Plasticity in the ABAQUS Finite Element Program. Cambridge, Massachusets: Harvard University; 1991; MECH-178.

[12] Asaro, Robert J. Micromechanics of Crystals and Polycrystals. Micromechanics in Applied Mechanics. 1983; 23:2-115.

[13] Tensile Tests, Specimens 5 mm for LISSAC. EMPA; 2001; Test Report, Nr. 201951/01.

[14] Nemat-Nasser, Sia and Hori, Muneo. Micromechanics: Overall Properties of Heterogeneous Materials. Amsterdan: North-Holland; 1993.

[15] Weyer, Stefan. Experimentelle untersuchung und mikromechanische Modellierung des Schädigungsverhaltens von Aluminiumoxid unter Druckbeanspruchung. Karlsruhe, Germany: Universität Karlsruhe; 2001.