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Vpliv zrnate strukture na elasto-plastični odziv polikristalnega skupka

The Effect of Grain Structure on the Elastic-Plastic Response of a Polycrystalline Aggregate

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Ena od ključnih predpostavk klasične mehanike trdnin je idealiziranje nehomogene mikrostrukture materiala. Ob takšni predpostavki ne moremo natančno napovedati razlik med meritvami odziva različno velikih, a geometrijsko podobnih preskušancev (vpliv velikosti). Za določitev vpliva zrnate strukture na makroskopski odziv je predlagan postopek, ki modelira elasto-plastično obnašanje materiala na mezoskopski ravni. Glavna zamisel je razdelitev trdnine na posamezne dele. Obravnava makroskopskega elementa je razdeljena na modeliranje naključne kristalne strukture (uporaba Voronojevega mozaika in naključne usmerjenosti kristalne rešetke) ter izračun napetostnega oziroma deformacijskega polja. Glavni namen prispevka je ocena najmanjše velikosti polikristalnega skupka, nad katero se makroskopska nehomogenost zrnate strukture danega materiala porazgubi in zato ni pričakovati, da bi povzročala opaznejši vpliv velikosti.

(Ključne besede: mikrostrukture materialov, strukture zrnate, skupki polikristalni, polja deformacijska)

One of the key assumptions of classical continuum mechanics is the idealization of the non-homogenous microstructure of a material. With this assumption in mind, the differences between measured responses of specimens that are different in size but geometrically similar (size effect) cannot be predicted accurately. A numerical approach, which models elastic-plastic behavior on the mesoscopic level, is proposed to determine the effect of the polycrystalline grain structure on the macroscopic response. The main idea is to divide the continuum into a set of sub-continua. The analysis of the macroscopic element is divided into modeling the random grain structure (using Voronoi tessellation and the random orientation of crystal lattice) and the calculation of the strain/stress field. The main purpose of the paper is to estimate the minimum size of the polycrystalline aggregate above which the macroscopic inhomogeneity of the grain structure of a given material vanishes and is therefore not expected to cause significant size effects.

(Keywords: microstructure, grain structures, polycrystalline aggregate, strain-stress fields)

0 UVOD

V zadnjih letih je bilo veliko naporov vloženih v določanje mehanskih lastnosti polikristalnih skupkov različnih velikosti. Klasična mehanika trdnin predpostavlja, da so lastnosti materiala homogene prek celotnega spektra tipičnih dolžin in zato neodvisne od velikosti preskušanca. Razlik med meritvami odziva različno velikih, a geometrijsko podobnih preskušancev (vpliv velikosti) tako ne moremo natančno napovedati [1]. To je v nasprotju z eksperimentalnimi podatki, ki kažejo, da velikost preskušanca lahko pomembno vpliva na obnašanje materiala. Tako se je pojavilo več postopkov, ki numerično modelirajo nehomogen material na mezoskopskem nivoju. Pri tem so se uveljavili postopki, ki poskušajo napovedati obnašanje polikristalnih skupkov z upoštevanjem zrnate

0 INTRODUCTION

A lot of efforts were made during the past few years to determine the mechanical properties of polycrystalline aggregates of different sizes. Classical continuum mechanics assumes the material properties to be homogeneous over the entire length scale, and therefore not dependent on the specimen size. The differences between the measured responses of specimens, which are different in size but geometrical similar (size effect), cannot be predicted accurately [1]. This is in opposition to experimental data, which shows that specimen size may contribute significantly to the material behavior. As a result, some approaches have appeared for the numerical modeling of inhomogenous material on the mesoscopic level. The emphasis was on approaches that predict the behavior of polycrystalline aggregates with a consideration of the

strukture materiala [2]. Dosedanji postopki so bili bolj usmerjeni na elastično območje, postopki mezoskopskega modeliranja plastičnih deformacij pa so se razvili šele v zadnjem desetletju.

Nehomogenost polikristalnih materialov sega prek celotnega spektra tipičnih dolžin [3]. Za potrebe prispevka je spekter tipičnih dolžin razdeljen na mikroskopsko raven (raven posameznih atomov s tipično velikostjo do 1 nm), mezoskopsko raven (kristalna zrna s tipično velikostjo 10 do 100 μm) in makroskopsko raven (strojni elementi s tipično velikostjo nad 10 mm). Za vsako raven obstajajo posebne konstitutivne enačbe, ki popišejo obnašanje materiala na tej ravni, pri čemer so konstitutivne enačbe na nižjih ravneh (mikroskopskih in mezoskopski) praviloma preprostejše [4].

Postopki, ki poskušajo pomanjkljivosti klasične mehanike trdnin zaobiti z numeričnim modeliranjem materiala na nižjih ravneh, so omejeni z računalniškimi zmogljivostmi. Za numerično modeliranje makroskopskih objektov na mikroskopski ravni je namreč potrebno izjemno veliko število gradnikov (npr. atomov) oziroma preračunov z ustreznimi konstitutivnimi enačbami. Razlike v tipičnih velikostih gradnikov mikroskopskih, mezoskopskih in makroskopskih ravni znašajo tudi nekaj velikostnih razredov (npr. v 1 mm^3 jekla je približno 10^{20} atomov [5]), kar seveda močno omejuje uporabnost takšnih postopkov (npr. [6] in [7]).

Za določitev vpliva polikristalne zrnate strukture na makroskopski odziv smo uporabili numerični postopek [8], ki modelira elasto-plastično obnašanje materiala na mezoskopski ravni. Glavna zamisel je razdelitev trdnine (npr. polikristalnega skupka) na posamezne dele (npr. kristalna zrna). Skupne lastnosti takšnega polikristalnega skupka so posledica lastnosti naključno oblikovanih in usmerjenih kristalnih zrn ter njihovega števila v polikristalnem skupku. Obravnava makroskopskega elementa je razdeljena na modeliranje naključne kristalne strukture (Voronojev mozaik in naključna usmerjenost kristalne rešetke) ter izračun napetostnega oziroma deformacijskega polja (uporaba preprostih fizikalnih modelov).

Uporabljena je metoda končnih elementov (programski paket ABAQUS [9]), ki se je v dosedanjih raziskavah izkazala kot primerna za računsko vrednotenje vedenja polikristalnih skupkov na mezoskopski ravni ([2] in [10]). Zaradi računske zahtevnosti je analiza omejena na 2D modele. V analizi so uporabljeni podatki jekla za reaktorske tlačne posode 22 NiMoCr 3 7, ki ima bainitno mikrostrukturo s telesno osrednjeno kubično mrežo.

Poglavitni namen prispevka je ocena najmanjše velikosti polikristalnega skupka, nad katero makroskopska nehomogenost zrnate strukture danega materiala izgine in zato ni pričakovati, da bi povzročala opaznejši vpliv velikosti.

material microstructure [2]. Previous approaches concentrated more on the elastic behavior, with the mesoscopic approaches to the modeling of plastic behavior tending to be developed in the past decade.

The inhomogeneity of materials stretches over the whole length scale [3]. For the purpose of this paper the length scale was divided into the microscopic level (of single atoms, with a typical size up to 1 nm), the mesoscopic level (crystal grains, with a typical size of 10 to 100 μm) and the macroscopic level (machine parts, with a typical size over 10 mm). Each level has distinctive, constitutive equations, which describe the material behavior on that level. The constitutive equations of the lower levels (e.g. microscopic and mesoscopic) are usually simpler [4].

Approaches that try to avoid the imperfections of classical continuum mechanics by numerical modeling of material on the lower levels are limited by computational capabilities. For the numerical modeling of macroscopic parts on the microscopic level an exceptionally large number of components (e.g. atoms) or calculations with appropriate constitutive equations is needed. The typical sizes of components on microscopic, the mesoscopic or the macroscopic levels differ by orders of magnitude (e.g. 1 mm^3 of steel is made of about 10^{20} atoms [5]). This certainly severely limits the use of microscopic models to model macroscopic parts (e.g. [6] and [7]).

A numerical approach [8], which models the elastic-plastic behavior of polycrystalline aggregate on the mesoscopic level, was used to determine the effect of the grain structure on the macroscopic response. The main idea is to divide continuum (e.g. a polycrystalline aggregate) into a set of sub-continua (grains). The overall properties of the polycrystalline aggregate are the outcome of the properties of randomly shaped and oriented grains and their number in the polycrystalline aggregate. An analysis of the macroscopic element is divided into modeling the random grain structure (Voronoi tessellation and the random orientation of the crystal lattice) and a calculation of the strain/stress field (use of simple physical models).

The finite-element method (program code ABAQUS [9]), which has proved to be suitable for the numerical modeling of the behavior of polycrystalline aggregate at the mesoscopic level, is used ([2] and [10]). The analysis is limited to two-dimensional models due to the limited computational capabilities. The material parameters for a steel pressure vessel made of 22 NiMoCr 3 7, with a bainitic microstructure and body-centred-cubic crystals are used in the analysis.

The main goal of the paper is to estimate the minimum polycrystalline aggregate size, above which the macroscopic inhomogeneity of the grain structure of a given material vanishes, and is therefore not expected to cause significant size effects.

1 TEORETIČNI MODEL

Osnovne predpostavke teoretičnega modela so:

- Za modeliranje naključne polikristalne strukture je uporabljen Voronojev mozaik.
- Vsako kristalno zrno je predpostavljeno anizotropno elastično z naključno usmeritvijo kristalne rešetke.
- Model plastičnosti predpostavlja, da plastična deformacija nastane zaradi zdrsa po vnaprej določenih ravninah zdrsa kristalne rešetke. Ravnine in smeri zdrsa so določene z usmeritvijo kristalne rešetke, ki se od zrna do zrna razlikuje (naključna usmeritev).

1.1 Voronojev mozaik

Zamisel Voronojevega mozaika je šele od nedavnega obsežneje uporabljena v znanosti o materialih, še posebej za modeliranje naključnih mikrostruktur, na primer skupki zrn v polikristalih, vzorci medkristalnih razpok in kompozitni materiali ([10] in [11]). Voronojev mozaik sestavlja celična struktura, ki jo dobimo iz Poissonovih točk tako, da postavimo mejo med celicama pravokotno na zveznico (na polovico razdalje) med sosednjima Poissonovima točkama. Rezultat je množica konveksnih teles (slika 1), ki popolnoma zapolni tako razdeljeno ravnino. Vsi v tem prispevku uporabljeni mozaiki so bili izdelani s programom VorTess [12].

1.2 Anizotropna elastičnost

Jeklo za reaktorske tlačne posode 22 NiMoCr 3 7 ima telesno osrednjeno kubično mrežo s precej izrazitim ortotropnim elastičnim odzivom. Predpostavljeno je, da se monokristal odziva kot

1 THEORETICAL MODEL

The basic assumptions of the theoretical model are:

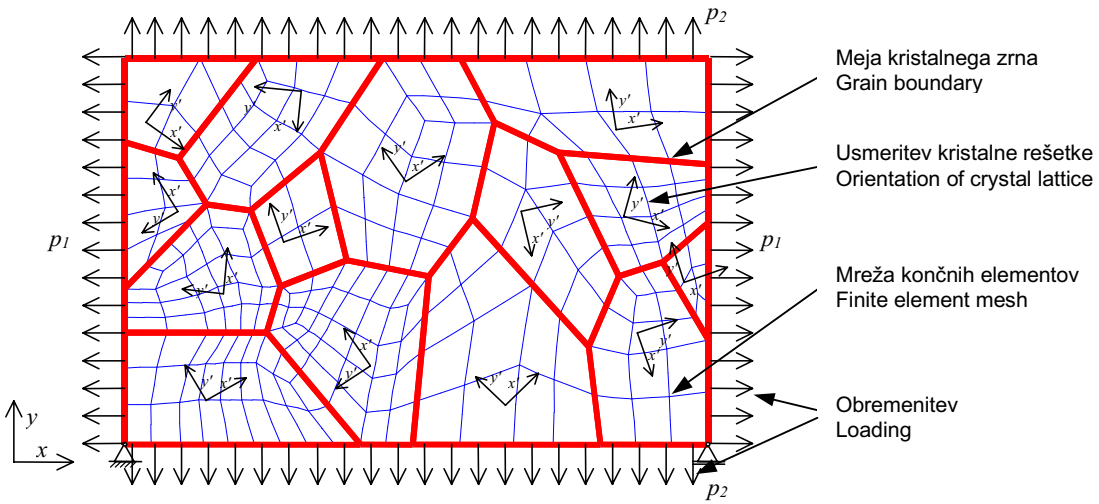
- The random polycrystalline structure is represented by a Voronoi tessellation.
- Each grain is assumed to be anisotropically elastic with a random orientation of the crystal lattice.
- The model of plasticity assumes that the plastic deformation is caused by crystalline slip on predefined slip planes of the crystal lattice. The slip planes and the direction are defined by the orientation of the crystal lattice, which differs from grain to grain (random orientation).

1.1 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 ([10] and [11]). A Voronoi tessellation represents a cell structure constructed from a Poisson point process by introducing planar cell walls perpendicular to the lines connecting neighboring points (at half point). 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 called VorTess [12].

1.2 Anisotropic elasticity

Pressure-vessel steel, 22 NiMoCr 3 7, has a body-centered-cubic crystal lattice with a rather pronounced orthotropic elasticity. Each crystal grain is assumed to behave as a continuum. The



Sl. 1. *Polikristalni skupek*
Fig. 1. *Polycrystalline aggregate*

trdnina, pri čemer zanj velja posplošeni Hookov zakon [13]:

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

kjer σ_{ij} pomeni tenzor napetosti 2. reda, C_{ijkl} tenzor togosti 4. reda in ε_{kl} tenzor specifičnih deformacij 2. reda. Elastične lastnosti polikristalnega skupka so popolnoma določene z lastnostmi in medsebojnim delovanjem posameznih monokristalov. Elastični materialni parametri so pridobljeni iz literature za železo α s telesno osrednjeno kubično mrežo ([14] in [15]). Predpostavljeno je, da majhne količine legirnih elementov ne vplivajo na elastično togost in podajnost monokristalov [15]. Uporabljeni so naslednji elastični snovni parametri: C_{iiii} = 230 GPa, C_{iijj} = 135 GPa in C_{ijij} = 117 GPa [15].

1.3 Kristalna plastičnost

Kristalna plastičnost predpostavlja, da je plastična deformacija posledica zgolj zdrsa kristalnih ravnin. Predpostavljeno je, da je Schmidova napetost (strižna napetost v sistemu zdrsa) gonilna sila zdrsa [16]. Sistem zdrsa je določen s kombinacijo ravnine (določena z normalo $m_i^{(\alpha)}$) in smerjo zdrsa ($s_i^{(\alpha)}$) znotraj kristalne rešetke. Telesno osrednjena kubična mreža ima tri družine ravnin zdrsa: {110}, {112} in {123} ter eno družino smeri zdrsa: <111>, kar pomeni 48 možnih sistemov zdrsa [17]. Osnovni zakon kristalografskega zdrsa se glasi:

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

kjer $\dot{\sigma}_{ij}$ pomeni časovni odvod tenzorja napetosti, $\dot{\varepsilon}_{kl}$ je časovni odvod tenzorja specifične deformacije, $\dot{\varepsilon}^p_{kl}$ časovni odvod tenzorja plastične specifične deformacije in $\dot{\gamma}^{(\alpha)}$ hitrost zdrsa sistema zdrsa α.

Plastičnost neodvisno od hitrosti deformacije lahko obravnavamo kot mejni primer plastičnosti, odvisne od hitrosti deformacije [16]. Hitrost zdrsa $\dot{\gamma}^{(\alpha)}$ je določena z ustrezno Schmidovo napetostjo $\tau^{(\alpha)}$:

$$\dot{\gamma}^{(\alpha)} = \dot{a}^{(\alpha)} \left(\frac{\tau^{(\alpha)}}{g^{(\alpha)}} \right) \left(\left| \frac{\tau^{(\alpha)}}{g^{(\alpha)}} \right| \right)^{n-1} \quad (3),$$

pri čemer so $\dot{a}^{(\alpha)}$ referenčna stopnja strižne napetosti, n je občutljivostni parameter strižne napetosti in $g^{(\alpha)}$ trenutno stanje utrjevanja monokristala. V limiti, ko se n približuje neskončnosti, enačba (3) ustreza enačbi za material, neodvisen od hitrosti deformacije. Trenutno stanje deformacijskega utrjevanja monokristala $g^{(\alpha)}$ je določeno iz hitrosti deformacijskega utrjevanja $\dot{g}^{(\alpha)}$:

$$\dot{g}^{(\alpha)} = \sum_\beta h_{\alpha\beta} \dot{\gamma}^{(\beta)} \quad (4),$$

kjer $h_{\alpha\beta}$ pomeni modul utrjevanja. Modul utrjevanja je obravnavalo več avtorjev ([16] in [18]), vsi pa imajo

constitutive relations are given by the generalized Hooke's law [13]:

where σ_{ij} represents the stress tensor of the 2nd rank, C_{ijkl} the stiffness tensor of the 4th rank, and ε_{kl} the strain tensor of the 2nd rank. The elastic properties of the polycrystalline aggregate are completely defined by the properties of, and interaction between, the crystal grains. The material parameters for the elasticity are obtained from the literature for α-Fe with a body-centered-cubic crystal lattice ([14] and [15]). It is assumed that small amounts of alloying elements do not change the elastic stiffness/compliance of a crystal grain significantly [15]. The following elastic material parameters were used C_{iiii} = 230 GPa, C_{iijj} = 135 GPa and C_{ijij} = 117 GPa [15].

1.3 Crystal Plasticity

Crystal plasticity assumes that plastic deformation is the result of crystalline slip only. It is assumed that crystalline slip is driven by Schmid stress (resolved shear stress). The slip system by a defined with combination of a slip plane (defined by its normal $m_i^{(\alpha)}$) and a slip direction ($s_i^{(\alpha)}$) within the crystal lattice. A body-centered-cubic crystal lattice has three families of slip planes – {110}, {112} and {123} – and one family of slip directions, <111>, which accounts for 48 possible slip systems. The basic law of crystalline slip is:

where $\dot{\sigma}_{ij}$ is the stress-rate tensor, $\dot{\varepsilon}_{kl}$ is the strain-rate tensor, $\dot{\varepsilon}^p_{kl}$ is the plasticity strain-rate tensor and $\dot{\gamma}^{(\alpha)}$ is the slipping rate of the α-th slip system.

Rate-independent plasticity may be treated as the limit of rate-dependent visco-plasticity [16]. The slipping rate $\dot{\gamma}^{(\alpha)}$ is determined by the corresponding Schmid stress $\tau^{(\alpha)}$ as:

where $\dot{a}^{(\alpha)}$ is the reference strain rate, n is the strain-rate sensitivity parameter and $g^{(\alpha)}$ is the current strain-hardened state of the crystal. In the limit as n approaches infinity, eq. (3) approaches that of a rate-independent material. The current strain-hardened state of the monocrystal $g^{(\alpha)}$ can be derived from the strain-hardened rate $\dot{g}^{(\alpha)}$:

where $h_{\alpha\beta}$ are the slip-hardening moduli. Other authors have dealt with hardening moduli ([16] and [18]), with

za osnovo izkustvene modele. V naši raziskavi smo uporabili Peirce et al. [19] ter Asaro ([18] in [20]), zakon o utrjevanju materiala, ki za izračun modula utrjevanja uporablja naslednji enačbi:

$$h_{\alpha\alpha} = h(\gamma) = h_0 \ \ \mathrm{sech}^2 \left| \frac{h_0 \gamma}{\tau_S - \tau_0} \right| \ \text{in/and} \ \ h_{\alpha\beta} = q h(\gamma) \quad (\alpha \neq \beta) \tag{5},$$

kjer so: h_0 začetni modul utrjevanja, τ_0 meja tečenja, ki je enaka začetni vrednosti trdnosti materiala $g^{(\alpha)}(0)$, τ_S je mejna napetost, nad katero se začenjajo velike plastične deformacije, γ kumulativni zdrs in q faktor utrjevanja. Plastični snovni parametri so pridobljeni iz literature za kristalno plastičnost, neodvisno od hitrosti deformacije [17], in iz rezultatov nateznega preskusa obravnavanega jekla. Uporabljene so bile naslednje vrednosti: občutljivostni parameter strižne napetosti $n = 50$, referenčna hitrost strižne napetosti $\dot{a}^{(\alpha)} = 0{,}001$ s^{-1}, začetni modul utrjevanja $h_0 = 70$ MPa, mejna napetost velikih plastičnih deformacij $\tau_S = 15{,}5$ MPa, meja tečenja $\tau_0 = 155$ MPa in faktor utrjevanja $q = 1$.

Enačbe (2) do (5) so za uporabo z metodo končnih elementov podane v koračni obliki [16]. Te enačbe so v splošnem zelo toge [13]. Togost sistema narašča z naraščanjem števila sistemov zdrsa. Zaradi togosti potrebuje klasična računska shema zelo majhne korake (in dolge računske čase) za zagotovitev stabilnosti rešitve.

1. 4 Ocena velikosti reprezentativnega prostorninskega elementa

V literaturi se je za najmanjši vzorec nehomogene snovi, ki je makroskopsko homogena, uveljavil termin reprezentativni prostorninski element (RPE). Velja, da pri vzorcu nehomogene snovi, večjim od RPE, vpliv velikosti na makroskopskem nivoju ni opazen [13].

Velikost RPE polikristalnega skupka je določena s primerjavo makroskopskega tenzorja togosti C^*_{ijkl} in tenzorja podajnosti D^*_{ijkl}. Pri tem so makroskopske veličine povprečene po celotnem polikristalnem skupku. Za polikristalni skupek, večji od RPE, velja ([10] in [21]):

$$C^*_{ijkl} \cong \left(D^*_{ijkl} \right)^{-1} \tag{6}.$$

Enačba (6) v splošnem ne velja za polikristalne skupke, manjše od RPE. Obnašanje takšnih polikristalnih skupkov je odvisno od njihovih velikosti in makroskopskih robnih pogojev [13]: makroskopski tenzor togosti predpostavlja robni pogoj s predpisano napetostjo, makroskopski tenzor podajnosti pa robni pogoj s predpisanim pomikom. Z upoštevanjem razmerij med napetostmi in specifičnimi deformacijami (npr. enačba (1)), je enačbo (6) mogoče poenostaviti z uporabo makroskopskih napetosti ali specifičnih deformacij [22], npr.:

all of them basing their work on empirical models. The Peirce et. al. [19] and Asaro ([18] and [20]) hardening law is used in our research, which uses the following equations:

where h_0 is the initial hardening modulus, τ_0 is the yield stress, which equals the initial value of the current strength $g^{(\alpha)}(0)$, τ_S is the the break-through stress, where large plastic flow initiates, γ is the cumulative slip and q is the hardening factor. Material parameters for the plasticity are obtained from the literature for rate-independent crystal plasticity (e.g. [17]) and from the results of a standard tensile test of the selected material. 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, the yield stress $\tau_0 = 155$ MPa and the hardening factor $q = 1$.

For the use with the finite-element method, equations (2) to (5) are given in incremental form [16]. These equations are, in general, very stiff [13]. The stiffness of the system increases with the number of slip systems. Due to the stiffness the classical integration scheme needs very small incremental steps (and long computational times) to ensure solution stability.

1.4 Estimation of the representative volume element size

The minimum size of a mesoscopically inhomogenous material that is macroscopically homogenous is, in the literature, usually refered to as the representative volume element (RVE). For volumes of mesoscopically inhomogenous material larger than the RVE the size effect at the macroscopic level cannot be observed [13].

The RVE size is defined by a comparison of the macroscopic stiffness C^*_{ijkl} and the compliance tensors D^*_{ijkl}. The macroscopic quantities are averaged over the entire polycrystalline aggregate. For polycrystalline aggregate larger than RVE stands ([10] and [21]):

Equation (6) is, in general, not valid for polycrystalline aggregates smaller than RVE. The behavior of polycrystalline aggregates is governed by their size and the macroscopic boundary conditions [13]: the macroscopic stiffness tensor therefore assumes a stress-driven boundary condition, while the macroscopic compliance tensor assumes a displacement-driven boundary condition. With general relations between stresses and strains in mind (as for instance described in equation (1)), equation (6) can be simplified by using macroscopic equivalent stresses or strains [22], e.g.:

$$\left\langle \sigma_{eq_s} \right\rangle \cong \left\langle \sigma_{eq_d} \right\rangle \tag{7}.$$

Indeksa $_s$ in $_d$ označujeta robna pogoja s predpisano napetostjo oziroma pomikom. Tako poenostavljeno merilo je, navkljub poenostavitvam, dovolj dobra ocena za predstavitev ključne težnje [22]. Nekateri avtorji za določitev velikosti RPE uporabljajo ekstrapolacijo z upoštevanjem velikosti polikristalnega skupka [21]. Razmerje med makroskopskima tenzorjema togosti in podajnosti za polikristalni skupek se lahko izrazi kot [21]:

Indexes $_s$ and $_d$ denote the stress- and displacement-driven boundary conditions, respectively. This simplified condition is sufficient to present the crucial trends [22]. Some authors have used an extrapolation to estimate the RVE size. The extrapolation is based on the size of a polycrystalline aggregate [21]. The relation between stiffness and compliance tensors for that polycrystalline aggregate can be written as [21]:

$$C^*_{ijkl}.D^*_{klmn} = I_{ijmn} + O\left(V/V_{RVE}\right) \tag{8},$$

kjer V_{RVE} pomenijo velikost RPE, V velikost polikristala, manjšega od RPE in O oceno ostanka. Z upoštevanjem enačbe (7) in dejstva, da je število zrn i v polikristalnemu skupku sorazmerno njegovi velikosti, namesto enačbe (8) uporabimo:

where V_{RVE} represents the RVE size, V is the size of a polycrystalline aggregate smaller than RVE, and O is the estimate of the residuum. With equation (7) and the proportionality between the number of grains in the polycrystalline aggregate, and its size, in mind, one can use:

$$\frac{\left\langle \sigma_{eq_s} \right\rangle}{\left\langle \sigma_{eq_d} \right\rangle} = 1 + O\left(i/i_{RVE}\right) \tag{9}.$$

Ocenjujemo, da je RPE dosežen, ko je ocena ostanka O manjša od 1% (0,1%).

We estimate that RVE size is achieved when residuum O is smaller than 1% (0.1%).

2 REZULTATI

Predstavljeni so nekateri rezultati predlaganega računskega postopka. Predstavljeni so primeri makroskopskega odziva polikristalnih skupkov z različnimi usmeritvami kristalnih rešetk in robnimi pogoji.

2.1 Diagram σ-ε

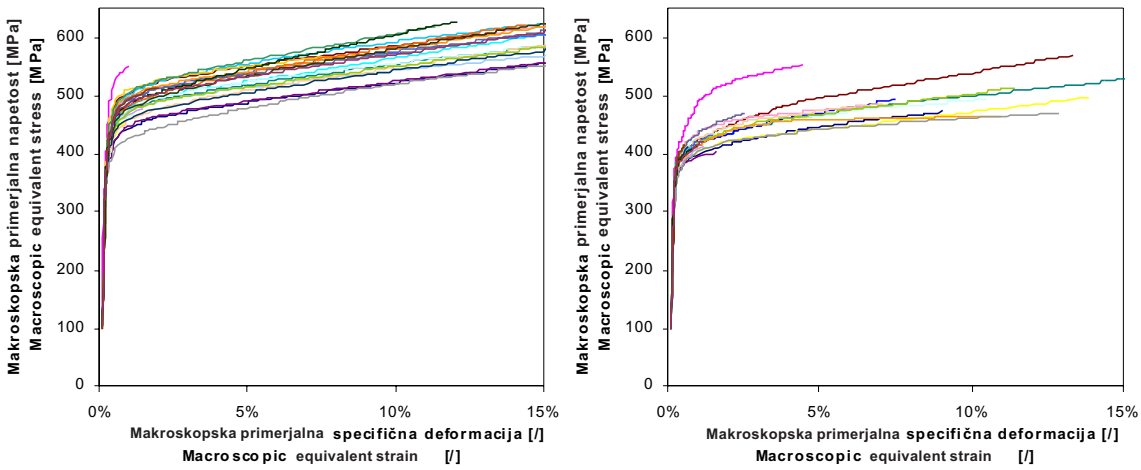
Na sliki 2 je predstavljena zveza med makroskopsko primerjalno (Misesovo) napetostjo in

2 RESULTS

The results of the proposed numerical approach are presented. Examples of the macroscopic response of polycrystalline aggregates with different orientations of the crystal lattice and boundary conditions are shown.

2.1 Stress-strain diagram

Figure 2 shows the relationship between the macroscopic equivalent (Mises) stress and the



Sl. 2. *Zveza med makroskopsko primerjalno napetostjo in primerjalno specifično deformacijo pri robnih pogojih s predpisanim pomikom (levo) in napetostjo (desno)*

Fig. 2. *A relationship between macroscopic equivalent stress and macroscopic equivalent strain with displacement (left) and stress driven boundary conditions (right)*

makroskopsko primerjalno specifično deformacijo za 30 različnih primerov naključnih usmeritev kristalnih rešetk za polikristalni skupek s 14 zrni (sl. 1). Predstavljena sta primera z robnimi pogoji s predpisanim pomikom in napetostjo.

Raztros krivulj zaradi različnih usmeritev kristalnih rešetk je razločno viden. V elastičnem območju krivulje močno sovpadajo, raztros meje tečenja pa je precejšen. Na robu predpisana napetost v povprečju povzroči bolj tog odziv. To je skupaj z že opisanimi težavami vzrok za manjše število analiziranih primerov.

2.2 Ocena velikosti RPE v elastičnem območju

Analize v elastičnem območju so bile opravljene na polikristalnih skupkih s 14, 23, 53, 110 in 212 zrni. Vsak polikristalni skupek je bil analiziran za 30 primerov naključne usmeritve kristalne rešetke (z na robu predpisano napetostjo oziroma pomikom). Analize so bile izvedene pri zunanji obremenitvi p_1 = 200 MPa in p_2 = 100 MPa (sl. 1). Rezultati so primerjani z analitično rešitvijo v izotropni trdnini s snovnimi lastnostmi: E = 210 GPa in ν = 0,29 [10].

Povprečne vrednosti so bile izračunane prek vseh 30 primerov usmeritev kristalne rešetke za vsak polikristalni skupek in robne pogoje. Rezultati so prikazani na sliki 3 (levo), pri čemer *s* in *d* označujeta robne pogoje s predpisano napetostjo oziroma pomikom, *ave* povprečno vrednost, naslednja številka pa število zrn v polikristalnem skupku. Prikazana je tudi analitična rešitev (makroskopska primerjalna specifična deformacija $\langle\varepsilon_{eq}\rangle$ = 0,0515 % in makroskopska primerjalna napetost $\langle\sigma_{eq}\rangle$ = 96,2 MPa). Opaziti je mogoče trend zmanjševanja raztrosa rezultatov ob večanju števila zrn v

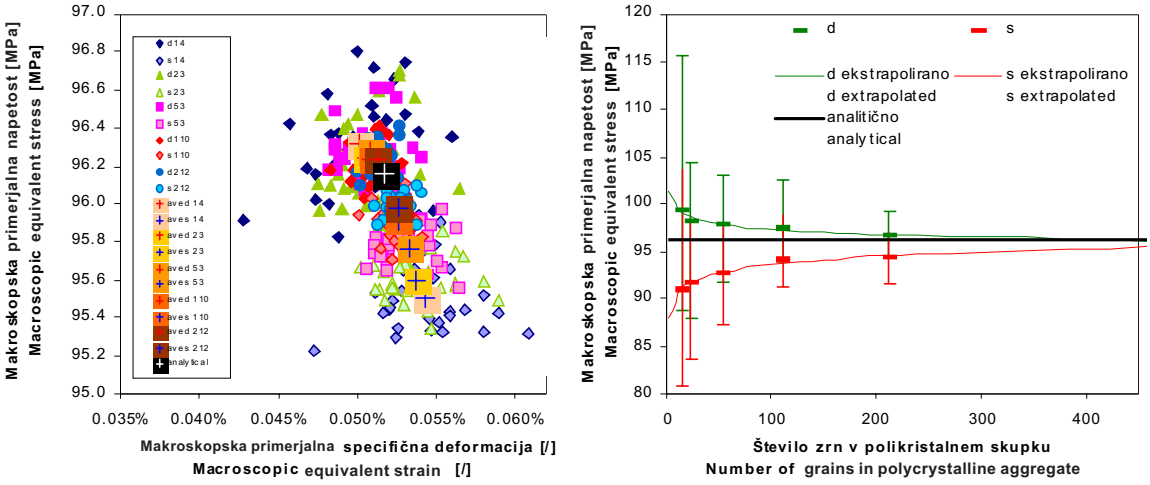
macroscopic equivalent strain for 30 cases with different orientations of crystal lattice for a 14-grains polycrystalline aggregate (Figure 1). Two cases with displacement and stress boundary conditions are presented.

The scatter of the curves due to the different orientations of the crystal lattice is clearly visible. The curves within the elasticity nearly coincide, with a distinctive scatter of yield points. The stress boundary condition causes a stiffer response. This, together with the difficulties mentioned above, is the cause for fewer analyzed cases.

2.2 Estimation of the RVE size within the elasticity

Analyses in the elasticity were carried out on polycrystalline aggregates with 14, 23, 53, 110 and 212 grains. Thirty different random orientations of crystal lattices with stress and displacement boundary conditions were analyzed for each polycrystalline aggregate. The analyses were carried out at macroscopic stress p_1 = 200 MPa and p_2 = 100 MPa (Figure 1). The results were compared with an analytical solution for an isotropic continuum with the material parameters: E = 210 GPa and ν = 0.29 [10].

Average values were calculated over 30 different random orientations of the crystal lattice for each polycrystalline aggregate and boundary condition. The results are shown in Figure 3 (left), where *s* and *d* refer to the stress and strain boundary conditions respectively, *ave* refers to the average values and the number following the abbreviation denotes the number of grains in the respective polycrystalline aggregates. The analytical solution (macroscopic equivalent strain $\langle\varepsilon_{eq}\rangle$ = 0.0515 % and macroscopic equivalent stress $\langle\sigma_{eq}\rangle$ = 96.2 MPa) is also shown. A tendency towards a reduced scatter of the results as the number of grains in the polycrystalline



Sl. 3. *Raztros makroskopskih primerjalnih napetosti in deformacij (levo) ter konvergenca makroskopske primerjlane napetosti v elastičnem območju (desno)*

Fig. 3. *Scatter of macroscopic equivalent strain/stress (left) and convergence of macroscopic equivalent stresses in elasticity (right)*

polikristlanem skupku. Povprečne vrednosti napetosti in specifičnih deformacij se pri povečevanju števila zrn v polikristalnem skupku bližajo analitični rešitvi.

Za oceno velikosti RPE v elastičnosti so bile izračunane makroskopske primerjalne napetosti pri makroskopski primerjalni specifični deformaciji $<\varepsilon_{eq}>$ = 0,0515 % (v skladu z analitično rešitvijo). Slika 3 (desno) prikazuje makroskopske primerjalne napetosti v odvisnosti od števila zrn v polikristalnem skupku pri robnih pogojih s predpisanim pomikom (označeno z *d*) in napetostjo (*s*). Ekstrapolacijske črte so narisane v skladu z enačbo (9). Iz razhajanja povprečnih vrednosti je razvidno, da RPE ni bil dosežen.

Nagibanje k analitični rešitvi in zmanjševanju razhajanja povprečnih vrednosti pri povečevanju števila zrn je jasno vidno. Velikost RPE je ocenjena iz enačbe (9). Z omejitvijo ostanka na 1 % znaša ocena velikosti RPE v elastičnem območju 280 zrn (kar ustreza polikristalnemu skupku velikosti približno 0,3 mm). Pri ostanku 0,1 % znaša predvidena velikost RPE 450 zrn (0,5 mm). Ugotovimo lahko, da so ocene v okviru pričakovanih iz literature (npr. [21]).

2.3 Ocena velikosti RPE v plastičnem območju

Analize v plastičnem območju so bile opravljene na polikristalnih skupkih s 14, 23, 53, in 110 zrni s po trideset primeri naključne usmeritve kristalnih rešetk (vsak primer z na robu predpisano napetostjo oziroma pomikom). Analize so bile izvedene pri zunanji obremenitvi p_1 = 1000 MPa in p_2 = 500 MPa (sl. 1).

V koračnih enačbah, ki popisujejo kristalno plastičnost, je bil uporabljen majhen računski korak (1 % celotne obremenitve), kar je povzročilo veliko časovno zahtevnost izračuna. Navkljub majhnemu računskemu koraku je zaradi togosti enačb prišlo do razhajanja in s tem do predčasnega končanja nekaterih analiz. Te težave niso dovoljevale, da bi bilo analiziranih vseh 30 primerov naključnih usmeritev kristalnih rešetk, toda razpoložljivi rezultati vseeno omogočajo, da predstavimo in pojasnimo bistvene težnje. V prihodnosti bo za izračun potreben še manjši korak ali drugačna računska shema [13].

Povprečne vrednosti so bile izračunane za vsak polikristalni skupek in robne pogoje. Rezultati so prikazani na sliki 4 (levo), pri čemer *s* in *d* označujeta robne pogoje s predpisano napetostjo oziroma pomikom, *ave* povprečno vrednost, naslednja številka pa število zrn v polikristalnem skupku. Videti je mogoče težnjo k zmanjševanju raztrosa rezultatov ob povečevanju števila zrn v polikristalnih skupkih. Povprečne vrednosti napetosti in specifičnih deformacij se pri

aggregate increases is visible. The average values of the stresses and the strains show a clear trend towards the analytical solution with an increasing number of grains in the polycrystalline aggregate.

To estimate the RVE size in elasticity, macroscopic equivalent stresses were taken at a 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 the number of grains in the polycrystalline aggregate for displacement- (denoted as *d*) and stress- (denoted as *s*) driven boundary conditions. The extrapolation lines are drawn in accordance with equation (9). From the scatter of the average values, one can conclude that the RVE has not been readred.

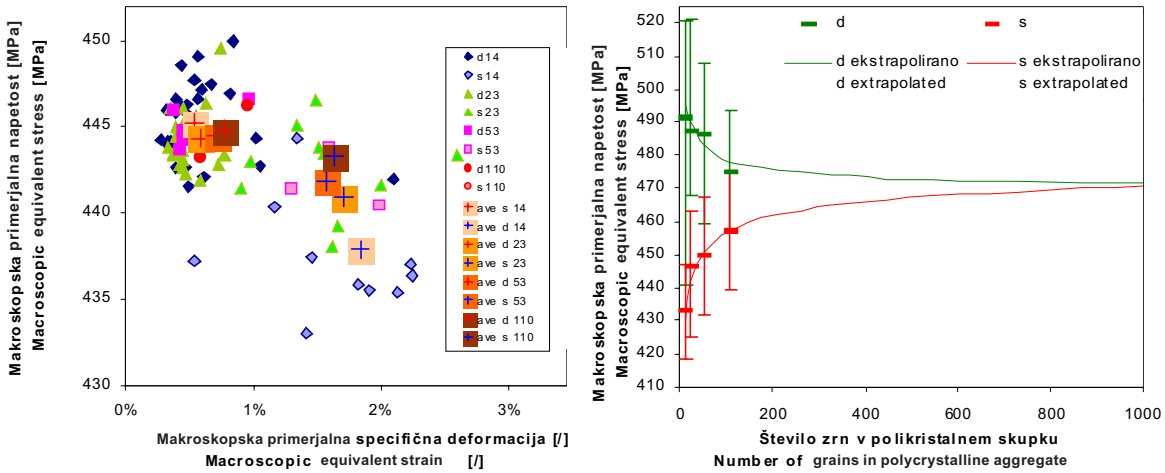
The trend towards the analytical solution and the decrease of scatter with an increasing number of grains is again clearly visible. The RVE size is estimated from equation (9). By limiting the residuum to 1 %, the estimation of the RVE size within the plasticity is 280 grains, which corresponds to a polycrystalline aggregate of about 0.3 mm in size. With a residuum of 0.1 %, the RVE size is estimated to be 450 grains (0.5 mm). One can conclude that the results are within those expected from the literature (e.g. [21]).

2.3 Estimation of RVE size within plasticity

Analyses in plasticity were carried out on a polycrystalline aggregate with 14, 23, 53, and 110 grains. Thirty different random orientations of crystal lattices and two boundary conditions (stress and displacement boundary conditions) were analysed for each polycrystalline aggregate. The analysis was performed at the macroscopic stress p_1 = 1000 MPa and p_2 = 500 MPa (Figure 1).

A small, incremental step (1 % of the total stress) was utilized in the incremental equations, which are used to describe the crystal plasticity. This caused a high computational demand for the analyses. Despite the small incremental step used, a divergence and therefore a premature end to some analyses appeared due to the equation stiffness. These difficulties did not allow for all 30 different randomly orientated crystal lattices to be analysed. Nevertheless, the available results enable us to show and explain the essential tendencies. An even smaller time step or unconventional time-integration schemes (e.g., [13]) should be used for analyses in the future.

The average values of the macroscopic equivalent stresses and strains were calculated for each polycrystalline aggregate and boundary condition. The results are shown in Figure 4 (left), where *s* and *d* refer to the stress and strain boundary conditions respectively, *ave* refers to average values and the number following the abbreviation denotes the number of grains in the respective polycrystalline aggregates. A tendency towards a reduced scatter of the results as the number of grains in the polycrystalline aggregates increases is visible. The average values of the



Sl. 4. *Raztros makroskopskih primerjalnih napetosti in specifičnih deformacij (levo) ter konvergenca makroskopske primerjalne napetosti v plastičnem območju (desno)*
Fig. 4. *Scatter of macroscopic equivalent strain/stress (left) and convergence of macroscopic equivalent stresses in plasticity (right)*

povečevanju števila zrn v polikristalnem skupku bližajo skupnemu povprečju.

Pri oceni velikosti RPE v plastičnem območju je bil uporabljen enak postopek kakor pri oceni v elastičnem območju. Makroskopske primerjalne napetosti so bile izračunane pri makroskopski primerjalni specifični deformaciji $<\varepsilon_{eq}> = 1$ %. Slika 4 (desno) prikazuje makroskopske primerjalne napetosti v odvisnosti od števila zrn v polikristalnem skupku pri robnih pogojih s predpisanim pomikom (označeno z *d*) in napetostjo (*s*). Ekstrapolacijske črte za povprečne vrednosti so narisane v skladu z enačbo (9). Razhajanje povprečnih vrednosti je večje kot 1 %, zato menimo, da RPE ni bil dosežen.

Nagibanje k skupnemu povprečju in zmanjševanju razhajanja povprečnih vrednosti pri povečevanju števila zrn je jasno vidno. Z omejitvijo ostanka na 1 % ocena velikosti RPE v plastičnem območju znaša 750 zrn (kar ustreza polikristalnemu skupku velikosti približno 0,6 mm). Pri ostanku 0,1 % znaša načrtovana velikost RPE nad 1000 zrn (0,7 mm).

3 SKLEP

V prispevku je bil predstavljen računski postopek za modeliranje elasto-plastičnega odziva materiala, ki združuje najpomembnejše mezoskopske značilnost in združljivost s klasično mehaniko trdnin. Uporabljeno je bilo eksplicitno modeliranje naključne zrnate strukture. Zrna modeliramo kot monokristale z anizotropno elastičnostjo in kristalno plastičnostjo. Postopek je bil uporabljen za oceno velikosti RPE polikristalnega skupka, nad katero makroskopska nehomogenost zrnate strukture danega materiala izgine in zatorej ni pričakovati, da bi povzročala vpliv velikosti.

stresses and strains show a clear trend towards a common average value with an increasing number of grains in the polycrystalline aggregate.

The same approach to estimate the RVE size as in elasticity was used. The macroscopic equivalent stresses were taken at the macroscopic equivalent strain of $<\varepsilon_{eq}> = 1$%. Figure 4 (right) shows the macroscopic equivalent stresses and scatter depending on the number of grains in a polycrystalline aggregate for displacement- (denoted as *d*) and stress- (denoted as *s*) driven boundary conditions. The extrapolation lines for the average values are drawn in accordance with equation (9). The scatter of the average values is larger than 1 %, therefore one can conclude that the RVE has not been achieved.

A tendency towards a common average value and a smaller scatter of average values, as the number of grains increases, is clearly visible. By limiting the residuum to 1 %, the RVE size within the plasticity is estimated to 750 grains (which corresponds to a polycrystalline aggregate of around 0.6 mm in size). With a residuum of 0.1 %, the RVE size is estimated to be above 1000 grains (0.7 mm).

3 CONCLUSION

A numerical approach that models the elastic-plastic material response was presented in this paper. The approach combines the most important mesoscale features and compatibility with the conventional continuum mechanics. Explicit modeling of the random grain structure was used. The grains were regarded as monocrystals (modeled with anisotropic elasticity and crystal plasticity). The approach was used to estimate the RVE size of a polycrystalline aggregate above which macroscopic inhomogeneity disappears and is therefore not expected to cause size effects.

Naključna zrnata struktura je vzrok za vpliv velikosti v polikristalnih skupkih, manjših od RPE. Velikost RPE v elastičnem območju je 280 zrn, kar ustreza vzorcu velikosti približno 0,3 mm. Velikost RPE v plastičnem območju je 750 zrn, kar ustreza vzorcu velikosti približno 0,6 mm. Oba podana primera sta izračunana ob predpostavki 1 % ostanka. Dobljeni rezultati so v skladu z rezultati iz literature. Predstavljen računski postopek dobro popisuje vplive zrnate strukture na elasto-plastičen odziv polikristalnega materiala.

V prihodnosti predvidevamo razširitev modela, ki bo vključeval razvoj poškodovanosti materiala in pospešitev izračuna (izdelava drugačne računske časovne sheme).

The random grain structure is the cause for size effects in polycrystalline aggregates smaller than the RVE. The RVE size within elasticity is estimated to be 280 grains, which corresponds to a specimen of about 0.3 mm in size. The RVE size within plasticity is estimated to be over 750 grains, which corresponds to a specimen of about 0.6 mm in size. Both cases were calculated with a residuum of 1% in mind. The proposed numerical approach is suitable for describing the effects of the grain structure on the elastic-plastic response of a polycrystalline aggregate.

Broadening of the approach, which will include the development of damage to be material and speeding up of the calculation (integration of different time-integration scheme) is foreseen in the future.

4 LITERATURA
4 REFERENCES

[1] Needleman, A. (2000) Computational mechanics at the mesoscale. *Acta Materialia*. 48, 105-124.

[2] Watanabe, O., H. M. Zbib, and E. Takenouchi (1998) Crystal plasticity, micro-shear banding in polycrystals using Voronoi tessellation. *International Journal of Plasticity.* 14(8), 771-778.

[3] Kröner, E. (1986) Statistical modelling. in: Gittus, John and Zarka, Joseph, Editors. Modelling small deformations of polycrystals. *Elsevier Applied Science*; 229-291.

[4] Gittus, J. and J. Zarka (1986) Modelling small deformations of polycrystals. London, *Elsevier*.

[5] Frost, H. J. and M.F. Ashby (1982) Deformation-mechanism maps. *Pergamon Press*; ISBN, 0-08-029338-7.

[6] Hafner, J. (2000) Atomic - scale computational materials science. *Acta Materialia*. 48, 71-92.

[7] Parker, A. (1999) Predicting material behavior from the atomic level up. *Science and Technology Review.* (6), 22-25.

[8] Kovač, M. Influence of microstructure on development of large deformations in reactor pressure vessel steel. Ljubljana: University of Ljubljana.

[9] Hibbit, Karlsson & Sorensen Inc. ABAQUS/Theory Manual, Version 6.2. Pawtucket, R.I., USA: Hibbit (2001) *Karlsson & Sorensen Inc*.

[10] Cizelj, L. and M. Kovač (2001) Constitutive models for the elastic-plastic polycrystalline aggregate with stohastic arrangement of grains. Rev 0. Ljubljana, *Institut Jožef Stefan;* IJS-DP-8334.

[11] Aurenhammer, F. (1991) Voronoi diagrams - a survey of a fundamental geometric data structure. *ACM Computing Surveys*. 23(3), 345-405.

[12] Riesch-Oppermann, H. (1999) VorTess, generation of 2-D random poisson-Voronoi mosaics as framework for the micromechanical modelling of polycristalline materials. Karlsruhe, Germany, *Forschungszentrum Karlsruhe*; Report FZKA 6325.

[13] Nemat-Nasser, S. and M. Hori (1993) Micromechanics: overall properties of heterogeneous materials. Amsterdam: North-Holland.

[14] Nye, J. F. (1985) Physical properties of crystals. Oxford, *Clarendon Press*.

[15] Grimvall, G. (1999) Thermophysical properties of materials. Amsterdam: North-Holland.

[16] Huang, Y.(1991) A user-material subroutine incorporating single crystal plasticity in the ABAQUS finite element program. *Cambridge, Massachusetts, Harvard University*; MECH-178.

[17] Nemat-Nasser, S.; T. Okinaka, and L. Ni (1998) A physically-based constitutive model for BCC crystals with application to polycrystalline tantalum. *Journal of the Mechanics and Physics of Solids.* 46(6), 1009-1038.

[18] Asaro, R. J. (1983) Micromechanics of crystals and polycrystals. *Micromechanics in Applied Mechanics.* 23, 2-115.

[19] Peirce, D.; R.J. Asaro, and A. Needleman (1982) Material rate dependence and localized deformation in crystalline solids. *Acta Metallurgica*. 31, 1951.

[20] Asaro, R. J. (1983) Crystal plasticity. *Journal of Applied Mechanics.* 50, 921.

[21] Weyer, S. (2001) Experimentelle Untersuchung und mikromechanische Modellierung des Schädigungsverhaltens von Aluminiumoxid unter Druckbeanspruchung. Karlsruhe, *Germany, University of Karlsruhe*.

[22] Cizelj, L. ; M. Kovač, Z. Petrič, L. Fabjan, and B. Mavko (2002) Effects of grain structure on elastic-plastic behavior of polycrystalline aggregate. Rev 0. Ljubljana, *Institute Jožef Stefan;* IJS-DP-8547.

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