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ANISOTROPIC HARDENING OF MATERIALS BY NON-SHEARABLE PARTICLES

UTRDITEV ANIZOTROPNIH MATERIALOV Z DELCI

[1]Napo Bonfoh, [2]Sonnou Tiem, [1]Paul Lipinski

[1]Laboratoire de Fiabilité Mécanique (L.F.M.), Ecole Nationale d'Ingénieurs de Metz (E.N.I.M.), Ile du Saulcy, F 57045 Metz Cedex 01, France
[2]Ecole Nationale Supérieure d'Ingénieurs (E.N.S.I.), Université de Lomé, B.P. 1515 Lomé, Togo
bonfoh@enim.fr; sonnou.tiem@togotel.net.tg; lipinski@enim.fr

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A new description of the hardening of polycrystalline materials is proposed. This hardening is mainly induced by non-shearable particles. Anisotropic and kinematic hardening of this kind of material has been mentioned in a previous paper (Bonfoh et al., 2003). In contrast to this initial investigation, the proposed modified formulation introduces a non-linear hardening for the single crystal without particles and better renders the material behaviour at finite deformations. The micromechanical modelling is based on a two-level homogenization approach: a micro-mesoscopic transition is firstly performed to derive the equivalent behaviour of a single crystal containing a volume fraction of intra-crystalline particles. Then, a second transition to the macroscopic scale leads to the elastic-plastic behaviour of the polycrystalline material. The numerical results of the model are analysed in terms of the internal stress developed during plastic loading. The material behaviour, when subjected to a multiaxial loading, is also studied through the concept of the yield surface. Some other aspects, such as the influence of particles size, shape and volume fraction, are also investigated.

Key words: crystal plasticity, inhomogeneous material, residual stress, yield surface, kinematic hardening

Predložen je nov opis utrditve polikristalnih materialov. To utrditev povzročajo nestrižni delci. V prejšnjem delu je bila opisana anizotropična in kinematična utrditev materiala te vrste (Bonfoh in dr., 2003). Nasprotno od te začetne raziskave predložena modificirana formulacija uvaja nelinearno mikromehansko modeliranje za nanokristal brez delcev in bolje opisuje vedenje materiala pri končni deformaciji. Mikromehansko modeliranje temelji na približku dvostopenjske homogenizacije: mikro-mezoskopska tranzicija je uporabljena za opis ekvivalentnega vedenja monokristala, ki vsebuje neki prostorninski delež intrakristalnih delcev, nato pa tranzicija na makroskopsko merilo vodi v elasto- plastično vedenje polikristalnega materiala. Numerični rezultati modela so analizirani s stališča notranjih napetosti, ki nastanejo pri plastični obremenitvi. Vedenje materiala pri večosni obremenitvi je analizirano s stališča plastičnega popuščanja površine. Analizirani so tudi drugi vidiki, npr. vpliv velikosti oblike in prostorninskega deleža delcev.

Ključne besede: plastičnost kristala, nehomogen material, zaostale napetosti, plastično popuščanje površine, kinematična utrditev

1 INTRODUCTION

Most polycrystalline materials exhibit, at the microscopic level, some heterogeneities, such as foreign atoms or particles. These heterogeneities, which may appear in the form of a solid solution or second-phase particles, may be located either between the crystals or inside the single crystals of the polycrystalline materials. In the present study, only the latter heterogeneities are considered. These intra-crystalline particles, such as precipitates, interact with moving dislocations during the material's plastic flow and lead to a modification of the single-crystal hardening.

Some papers have been devoted to a description of the influence of intra-granular heterogeneities on the behaviour of polycrystalline materials: Schmitt et al (1996), Bochet et al (2001), Barbe et al. (2001) and Han et al. (2004). Recently, Reza et al (in press) has proposed a description of crystalline materials containing non-interacting elastic particles. Performed within a small strain formulation and confined to uniform elasticity, the authors propose a calculation of the additional work of deformation (strain energy) arising from plastic strain-field incompatibilities between the elastic-plastic matrix and the elastic particles.

In this work, a micromechanical description of a single crystal containing particles is developed through a micro-meso transition. First, a modified Schmidt's law and a new hardening matrix, taking into account the usual dislocation-dislocation interactions and also the interactions between dislocations and particles, are proposed. Next, a meso-macro transition using the self-consistent method developed by Lipinski et al. (1993, 1998) is applied to deduce the global response of the polycrystalline material. A comparison between the classical self-consistent predictions and the new approach is made. Special attention has been focused on the prediction of the yield surfaces and the residual stresses.

2 DESCRIPTION OF THE SINGLE CRYSTAL WITH PARTICLES

In this paper, single crystals are assumed to contain a certain volume fraction of ellipsoidal particles. Moreover, at the microscopic level, the single crystal is considered as a two-phase material: the elastic-plastic crystalline matrix with elastic particles. The plastic straining of the crystal results from the movements of dislocations on geometrically well-defined slip planes. The classical theory of single-crystal plasticity is adopted and Schmidt's law is valid.

At the crystalline level, the presence of non-shearable particles results in some incompatibilities of the strain field between the crystalline matrix and the particles. These incompatibilities are mainly due to the anisotropy of elastic behaviour and the heterogeneity of plastic straining between the matrix and the particles. The stress rate inside the crystalline matrix is then given by:

$$\dot{\sigma}^{\mathrm{m}} = \dot{\sigma}^{1} + \tilde{P} : \dot{\varepsilon}^{\mathrm{m}} \tag{1}$$

The last term $\tilde{P} : \dot{\varepsilon}^{\mathrm{m}}$, represents internal stresses arising from these incompatibilities, where the fourth-rank tensor $\tilde{P}$ is the polarisation tensor describing the evident interactions between the two phases evolving inside the heterogeneous grain. The expression of this tensor $\tilde{P}$ can be derived using classical models of the interactions problems of heterogeneous materials (Kröner, Mori-Tanaka, Self-consistent, etc.). In this study, the last of these is used, and this leads to:

$$\tilde{P} = f(\tilde{I} - \tilde{b}^{3}) : \tilde{l}^{I} (\tilde{I} - f\tilde{a}^{3})^{-1} \tag{2}$$

where $\tilde{a}^{3}$ and $\tilde{b}^{3}$ are, respectively, the strain- and stress-rate localisation tensors inside the particles, $\tilde{l}^{\mathrm{I}}$ is the tangent elastic-plastic moduli of the equivalent single crystal with particles.

Moreover, assuming the following relationship for the hardening of the single crystal without particles:

$$\tau_{cr}^{g} = \sum_{h=1}^{N} H^{gh} \dot{\gamma}^{h} \tag{3}$$

It is also possible to derive a kind of Schmidt law for the equivalent heterogeneous grain:

$$R^{g} : \left[(1-f)\tilde{I} + \tilde{P} : \tilde{s}^{m} (\tilde{I} - f\tilde{b}^{3}) \right] : \dot{\sigma}^{I} = \\ = \sum_{h=1}^{N} (H^{gh} - R^{g} : \tilde{P} : R^{h}) : (1-f) \dot{\gamma}^{h} \tag{4}$$

The first term appears as the resolved shear-stress rate for the equivalent grain I subjected to the $\dot{\sigma}^{I}$ stress rate, where the second one reveals a new form of hardening matrix:

$$\aleph^{gh} = H^{gh} - R^{g} : \tilde{P} : R^{h} \tag{5}$$

taking into account the initial dislocation-dislocation interactions through the matrix H^{gh} but also the interactions between the particles and the dislocations during their movements ($R^{g} : \tilde{P} : R^{h}$).

The description of the equivalent behaviour of the single crystal with particles is therefore completed by the expression of its tangent elastic-plastic properties:

$$\tilde{l}^{I} = \tilde{C}^{I} - \sum_{g=1}^{N} \sum_{h=1}^{N} \tilde{C}^{I} : R^{g} K^{gh} R^{h} : \tilde{U} : \tilde{C}^{I} \tag{6}$$

$$\tilde{U} = (1-f)\tilde{I} + \tilde{P} : \tilde{s}^{m} : (\tilde{I} - f\tilde{b}^{3}) \quad \text{and} \\ K^{gh} = (\aleph^{gh} + R^{g} : \tilde{U} : \tilde{C}^{I} : R^{h})^{-1} \tag{7}$$

The superscripts *m*, 3 and *I* are, respectively, related to the matrix (single crystal without particle), particles and the considered grain *I*.

After this first transition from local microscopic properties to the mesoscopic level, leading to the grain behaviour, a second transition, to the macroscopic level, is then performed to derive the equivalent properties of the polycrystalline material consisting of a large number of single crystals with particles.

3 NUMERICAL SIMULATIONS

The proposed model is applied to the simulation of the material's behaviour. The selected material is a SiC particulate-reinforced 5456 aluminium alloy matrix composite:

- Matrix material (aluminium): Young's modulus E_{m} = 73 GPa, Poisson's ratio ν_{m} = 0.33, and initial uniaxial yield stress σ_{y} = 230 MPa.
- Elastic properties of SiC particles: Young's modulus E_{p} = 485 GPa and Poisson's ratio ν_{p} = 0.2.

3.1 Material behaviour under monotonous loading

The selected material is subjected to a uniaxial tension in direction 1, and its macroscopic response in terms of stress–strain is depicted in **Figure 1**.

The plotted curves exhibit an evident hardening of the macroscopic behaviour with the volume fraction of particles, since the particles considered here are harder than the crystalline matrix. Moreover, this hardening is characterized by an increasing of the equivalent elastic threshold and a non-linear evolution in its elastic-plastic part. Since the initial hardening of the single crystal is assumed linear, this non-linear aspect results from the original amendments introduced in the proposed hardening model.

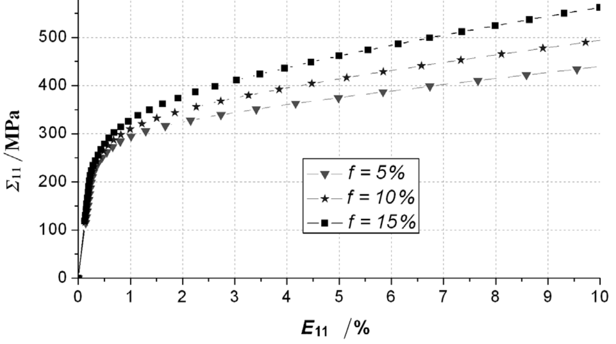

Figure 1: Macroscopic response for different volume fractions of particles

Slika 1: Makroskopski odgovor za različen volumenski delež delcev

In the present investigation, particles are non-shearable and during the plastic flow, dislocations bypass these obstacles with the Orowan-looping mechanism.

The initial critical shear stress on slip systems is influenced by particle interactions at the beginning of the plastic flow.

3.2 Yield surface

The material behaviour during multiaxial and non-proportional loads is analysed through the concept of a yield surface depicted in a stress plane. The yield surfaces proposed in this study are determined for a plastic offset of $E^p_{\mathrm{eq}} = \sqrt{2/3 E^p_{ij} E^p_{ij}} = 0.2$ %. The results in **Figure 2** correspond to the same material identified in the previous paragraph, and represent the macroscopic yield surface after two amounts of macroscopic equivalent strain (E_{eq} = 5 %, E_{eq} = 10 %) of a tensile pre-straining in direction 1.

These yield surfaces reveal:

- A vertex in the pre-straining direction, due to great inter and intra-granular residual stress being developed. These back stresses arising from incompatibilities of strain fields pointed out previously, increase the yield stress in this pre-loading direction.
- A flattening of the yield surface in the opposite direction to the pre-straining is also observed. This relative softening results from the decrease of the yield stress due to superimposed back stresses in this opposite direction.
- A hardening in directions transverse to the pre-loading is also visible.

Whatever the amount of pre-straining, the obtained equivalent behaviour exhibits a mixed anisotropic and kinematic hardening due to the intra-crystalline particles. A translation in the pre-straining direction combined with a non-homogeneous expansion of the yield surfaces is observed in **Figure 3**.

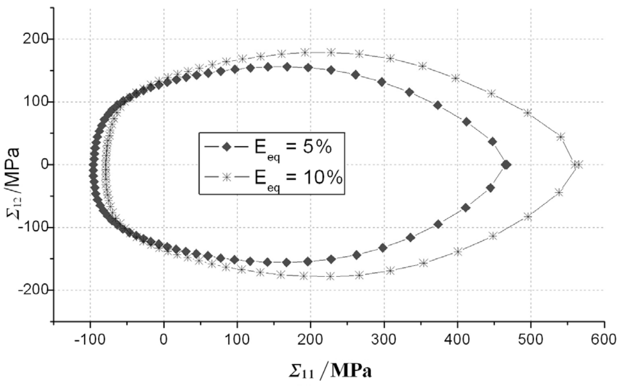

Figure 2. Macroscopic yield surfaces after a tensile pre-straining (in direction 1)

Slika 2: Makroskopsko plastično popuščanje površine po natezni predobremenitvi (v smeri 1)

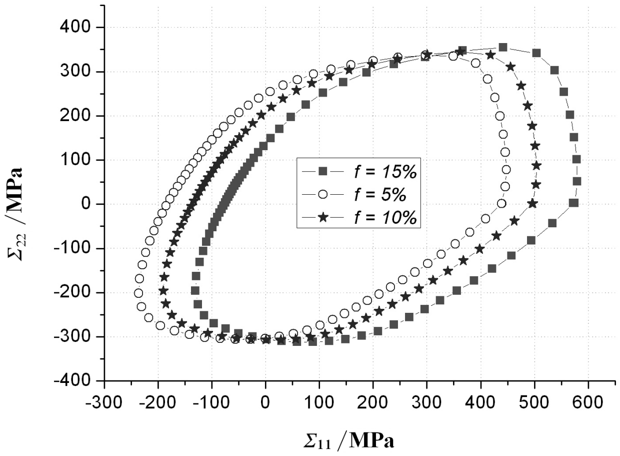

Figure 3: Material yield surfaces after a tensile pre-straining (in direction 1, E_{eq} = 10 %)

Slika 3: Površine plastičnega popuščanja materiala po natezni predobremenitvi (v smeri 1, E_{eq} = 10 %)

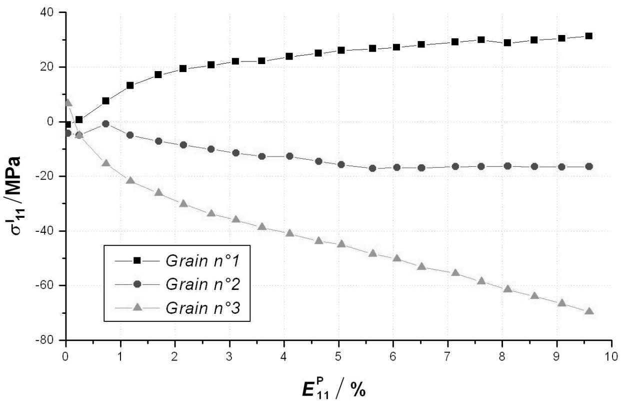

Figure 4: Residual stress inside particle after a tensile pre-straining (in direction 1)

Slika 4: Zaostale napetosti v notranjosti delca po natezni predobremenitvi (v smeri 1)

The presence of intra-crystalline-heterogeneities-induced internal stresses relates to the evident interactions between the latter and the dislocations during their movement. These internal stresses are developed both in the matrix and the particle, where a strong polarization is observed. After a pre-loading, leading to a significant permanent strain, followed by an unloading, there remains internal stresses called residual stresses. **Figure 4** depicts these residual stresses, developed inside particles for three selected grains of the polycrystalline material. Due to the elastic properties of the selected particles, these residual stresses seem to be relatively important for the macroscopic stress level. In contrast to previous investigation, their evolution is non-linear, because of the introduced new hardening matrix and differs from grain to grain.

4 CONCLUSION

The paper proposes a new formulation for the hardening of polycrystalline materials due to intra-crystalline heterogeneities such as precipitates. The suggested model takes into account internal stresses arising from the incompatibilities of the strain field between the crystalline elastic-plastic matrix and the purely elastic particles.

The observed hardening has been elucidated with numerical simulations of the behaviour response under monotonous, uni- and multi-axial loadings. The results, in terms of the yield surfaces and the internal stresses evolution with the volume fraction of the particle and also with the amplitude of specific pre-straining, are provided.

These internal stresses, characterised by a strong polarisation in the particles, leads to important interfacial stresses and the subsequent damage initiation by the particle's interface debonding. For this specific problem, a combined stress and energetic criterion is introduced, to take into account the particles' size effect, pointed out for the damage initiation in such materials.

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