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Analytical prediction of yield stress and strain hardening in a strain gradient plasticity material reinforced by small elastic particles

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ABSTRACT

The influence on macroscopic work hardening of small, spherical, elastic particles dispersed within a matrix is studied using an isotropic strain gradient plasticity framework. An analytical solution for strain hardening, i.e. the flow stress as a function of plastic strain, based on a recently developed model for initial yield strength is proposed. The model accounts for random variations in particle size and elastic properties, and is numerically validated against FE solutions in 2D/3D unit cell models. Excellent agreement is found as long as the typical particle radius is much smaller than the material length scale, given that the particle volume fraction is not too large (≤ 10%) and that the particle/matrix elastic mismatch is within a realistic range. Finally, the model is augmented to account for strengthening contribution from shearable particles using classic line tension models and successfully calibrated against experimental tensile data on an Al – 2.8wt% Mg – 0.16wt% Sc alloy.

1. Introduction

The effects of precipitated particles distributed within a bulk material is a well studied phenomenon. Pioneering works in the development of its theory are due to Orowan (1948) and Mott and Nabarro (1940), who explained the increase in yield strength using the concept of dislocations interacting with the particles. An excellent review on the subject of precipitation strengthening has been given by Ardell (1985). In essence, there are two types of interactions between a dislocation and a particle: either, the particle characteristics, such as size, coherency and crystallographic structure, are such that the dislocation will cut right through it, or the dislocation will bypass the particle without plastically deforming it. In addition, the bypassing process may be in the form of Orowan shear loops, or by thermally assisted motions such as cross slip or climb.

To model the strengthening and hardening of complex metallic material systems in general, a wide range of mechanisms have to be taken into account. These mechanisms contribute to the material flow stress by impeding dislocation motion and are typically due to grain boundaries, secondary phases, forest dislocations, solute atoms, and intrinsic dislocation glide resistance. Depending on the specific material system and processing, some of the above mechanisms will most likely dominate over the others which simplifies the modelling. How to superimpose contributions of relevance to flow stress is not trivial (Quereau et al., 2010; De Vaucorbeil et al., 2013). Since the 80’s, micro mechanical modelling of hardening based on dislocation–obstacle interaction has heavily relied on the work of Kocks, Mecking and Estrin (KME) (Mecking and Kocks, 1981; Estrin and Mecking, 1984; Kocks and Mecking, 2003), who propose a model for the evolution of dislocation density as a function of plastic strain. In essence, their model postulates that the accumulation rate of dislocation density is governed by the difference in rate of storage and annihilation. Given its versatile nature, this model can be modified to include a wide range of microstructure dependent mechanisms relevant to...
hardening. Once the governing equation for the dislocation density is established, its output typically enters the classic Taylor model of dislocation hardening. Some notable work on modelling the strengthening and hardening in metal systems containing precipitates include Russell and Brown (1972), Fazeli et al. (2008a), Myhr et al. (2010), Cheng et al. (2003), Deschamps and Brechet (1998) and Fribourg et al. (2011).

Another method of modelling the work hardening is to directly model the movement of each individual dislocation within a large group of dislocations under an applied macroscopic stress. Contributions using this framework, which is commonly referred to as Discrete Dislocation Dynamics (DDD), include Arsenlis et al. (2007), Koslowski et al. (2002), Santos-Güemes et al. (2020), Vattré et al. (2009) and Zbib et al. (2000).

Because of the apparent size effect in particle strengthening, cf. Kouzeli and Mortensen (2002), conventional continuum plasticity theories, e.g. $J_2$ plasticity, fall short in their predictive power due to their lack of an intrinsic length scale. However, strain gradient enriched continuum plasticity models offer a mean to resolve these small scale size effects by recognizing the close connection between the density of geometrically necessary dislocations (GNDs) and gradients in plastic strain. By adding the contributions from plastic strain gradients to the internal work and to the strain based measure of total dislocation density, a higher order theory framework with an intrinsic length scale can be constructed from conventional local theories of continuum plasticity, see e.g. Fleck and Hutchinson (1993), Fleck et al. (1994), Hutchinson and Fleck (1997), Fleck and Hutchinson (2001), Gudmundson (2004), Gurtin (2004), Gurtin and Anand (2005) and Fleck and Willis (2009b,a). For a thorough review on Strain Gradient Plasticity (SGP) theories, the reader is referred to the recent article by Voyiadjis and Song (2019), where also estimates of the intrinsic length scale as obtained from small scale testing are summarized (see also Evans and Hutchinson (2009)).

In most SGP theories, a division is made between energetic and dissipative contributions to higher order stresses and moments. For proportional loading however, as is considered in the present paper, the differences disappear. In recent years, the issue of so called elastic gaps at non-proportional loading has as well been discussed (Hutchinson, 2012; Fleck et al., 2014). Again, for proportional loading these effects do not appear.

Further, by also adding the work performed at an internal interface to the internal work, interface phenomena such as dislocation pile-ups and other grain boundary type features can be modelled. Relating dislocation movement and production to plastic strain, the higher order theories allow for restrictions, including a complete blockage, to the flow of dislocations through an internal boundary. Following the second law of thermodynamics, constitutive laws for the forces due to dislocation pile ups at internal interfaces, i.e. interface models, can be established by relating plastic strain to the moment stresses present in higher order SGP theories. These constitutive laws may be purely dissipative, purely energetic or a mix of both. The latter can be motivated through the fact that dislocation networks does store some elastic energy as they distort the lattice. Several thermodynamically consistent interface models within the framework of higher order isotropic SGP theories have been proposed over the years, e.g. Fleck and Willis (2009b), Fredriksson and Gudmundson (2005), Asgharzadeh and Faleskog (2021a), Dahlberg and Faleskog (2013) and Voyiadjis and Deliktas (2009).

Early attempts at studying particle reinforced metals using conventional $J_2$ plasticity continuum mechanics include Christman et al. (1989) and Bao et al. (1991). The authors in the latter reference found a simple relation for the elevation in yield stress for a metal reinforced by impenetrable rigid particles given by $\sigma_p = \beta \sigma_0 f$ where $\sigma_p$ is the yield stress in the matrix material, $f$ is the volume fraction of particles and $\beta$ is a parameter that depends on particle shape. Investigations using isotropic SGP theories to study above mentioned metals include Zhu et al. (1997), Dai et al. (1999), Yueguang (2001), Chen and Wang (2002), Xue et al. (2002), Liu et al. (2003), Qu et al. (2005) and Zhang et al. (2007).

In a recent work by Faleskog and Gudmundson (2021), an upper bound solution to predict the initial yield stress for the inhomogeneous inclusion problem was presented on the form

$$\sigma_{\text{UBS}}^0 = \frac{\sigma_0}{1 + \frac{3f\alpha\ell}{a}},$$

where $\ell$ denotes the material length scale of the matrix, $a$ the particle radius, $\Gamma$ an elastic constant calculated through Eshelby formalism and $\alpha$ a parameter related to the particle/matrix interface. This upper bound estimate is in close agreement with corresponding numerical full field solutions if the volume fraction of particles is less than 10%.

The main objective of the current work is to model the work hardening in a material hardened by a dispersion of small elastic particles. Specifically, an extension of the analytical model for initial yield stress by Faleskog and Gudmundson (2021) will here be sought to predict not only the initial yield stress but also the work hardening. The paper is structured as follows. In Section 2, the continuum model used for bulk and interface respectively is presented. Notably, a model to describe the effects of a strain softening internal interface is proposed based on the self energy of dislocation lines. In Section 3, an upper bound solution to the particle reinforced composite problem is presented. Section 4 contains simulation results validating the upper bound solution for a wide range of parameters. Results for a homogeneous distribution of spherical particles using an axi-symmetric model as well as a non uniform distribution in a 3D model are presented, and model limitations at high strain levels are discussed. The model is augmented to account for particle shearing in Section 5, and Section 6 contains comparisons between model predictions and experimental results. Finally, the article is summarized in Section 7.

2. Problem description

2.1. Model

The current investigation aims at predicting both yield strength and post yield strain hardening in a particle reinforced metal–matrix composite as measured in a standard tensile test. Essentially, the material dealt with is assumed to consist of small, smooth
The rate of dissipation can be written as

\[ \dot{\mathcal{W}} = \int_V \dot{\mathbf{E}} : \mathbf{E} \, dV. \]

2.3. Constitutive equations

In the volume considered, \( V \), particles occupy volume \( V_p \) and the matrix material \( V_m \). Sub-indices ‘m’ and ‘p’ will henceforth be used to distinguish between quantities in the matrix and particles, respectively. It should also be noted that a super-script ‘p’ will in the following denote plastic quantities. In addition to the volume fraction of particles \( f \), a representative (effective) value of particle size \( \bar{a} \) characterizes the microstructure of the material. For small volume fractions of particles, the interaction between particles can be neglected and hence the geometrical distribution of particles does not influence the predicted stress–strain behaviour. The influence of particles on strengthening depends on their size relative to the length parameter \( \ell \) of the matrix material and on their volume fraction, cf. Faleskog and Gudmundson (2021).

The proceeding analysis for bulk and particle–interface is based on energy considerations. If gradients of plastic strains influence the energetic state, corresponding conjugate higher order stress measures naturally arise. This is the essence of strain gradient plasticity theories. Higher order stresses, like moment stresses, may by themselves look unintuitive, but in the context of work per unit volume (or interface area) they have a clear physical meaning.

2.2. Variational formulation of strain gradient plasticity theory

The primary kinematic variables in the higher order, isotropic, small strain SGP theory by Gudmundson (2004) are displacements \( u_i \) and plastic strains \( \dot{\varepsilon}_{ij}^p \). These are related as

\[ \dot{\varepsilon}_{ij}^p = \frac{1}{2}(u_{ij,i} + u_{ij,i}), \quad \dot{\varepsilon}_{ij}^p = \varepsilon_{ij}^p + \dot{\varepsilon}_{ij}, \quad \varepsilon_{kk} = 0, \]

where \( \varepsilon_{ij} \) are the components of the total strain tensor and \( \dot{\varepsilon}_{ij}^p \) are the elastic strain components. As in conventional \( J_2 \)-plasticity theory, plastic incompressibility is assumed.

Mechanical equilibrium in absence of body forces in a solid of volume \( V \), with external/internal surfaces \( S_{ext}/S_f \), is expressed through the principle of virtual work as

\[ \int_V \left[ \sigma_{ij} \delta \varepsilon_{ij} + (q_{ij} - s_{ij}) \delta s_{ij} + m_{ijk} \delta \varepsilon_{ijk} \right] dV + \int_{S_f} \left[ \mathbf{M}^I \delta \varepsilon_{ij}^p \right] dS = \int_{S_{ext}} T_i \delta u_i + M_{ij} \delta \varepsilon_{ij}^p dS, \]

where \( \sigma_{ij} \) and \( s_{ij} = \sigma_{ij} - \delta_{ij} \sigma_{kk}/3 \) denote the components of the Cauchy stress tensor and its respective deviator while \( \delta_{ij} \) denotes the components of the Kronecker delta tensor. Including plastic strain and its gradients in Eq. (3) brings out their work conjugate stresses in this tensorial higher order theory. These are the micro stresses \( q_{ij} \) and the moment stresses \( m_{ijk} \), which are symmetric with respect to the first two indices. The moment stresses give rise to moment tractions \( M_{ij} \) on boundaries. Thus, on internal and external surfaces, the higher order moment tractions \( M_{ij}^I \) and \( M_{ij} \) naturally arise, both being work conjugate to \( \dot{\varepsilon}_{ij}^p \). In addition, \( T_i \) at the right-hand-side of (3) denote standard tractions.

2.3. Constitutive equations

In both matrix and particles, the elastic response is assumed to be linear and isotropic with Young’s modulus \( E_m \), \( E_p \) and Poisson’s ratios \( \nu_m \), \( \nu_p \), with shear modulus \( G_m = E_m/[2(1 + \nu_m)] \) and \( G_p = E_p/[2(1 + \nu_p)] \).

Assuming a purely dissipative bulk, i.e. the free energy in the bulk does not depend on plastic strains nor on the gradients thereof, the rate of dissipation can be written as

\[ \dot{D} = q_{ij} \dot{\varepsilon}_{ij} + m_{ijk} \dot{\varepsilon}_{ijk} = \mathbf{\Sigma} \dot{\mathbf{E}}^p \geq 0, \]
where the effective work conjugate measures of stress and plastic strain rate, respectively, have been introduced as

$$\Sigma = \left[ \frac{3}{2} a_{ij} a_{ij} + \frac{m_{ij} m_{ij}}{2\lambda} \right], \quad \dot{\Sigma} = \left[ \frac{1}{3} \left( \dot{e}_{ij}^p \dot{e}_{ij}^p + \dot{\epsilon}_{ij}^p \dot{\epsilon}_{ij}^p \right) \right]. \quad (5)$$

These measures reduce to those of standard $J_2$-plasticity quantities in absence of plastic strain gradients. Note that the inclusion of higher order terms in Eq. (5) necessitates a length parameter $\ell$, here viewed as a material constant. In the context of the current problem, $\ell$ sets the scale on which plastic strain gradients may influence the strengthening due to the build up of plastic strain gradients at the particle/matrix interface. Note that a length scale $\ell$ much smaller than other problem specific relevant length scales will remove the effects of strain gradients.

Constitutive rate equations satisfying Eqs. (4) and (5) are employed and defined as

$$\dot{\epsilon}_{ij}^p = \dot{\Sigma} \frac{a_{ij}}{\Sigma}, \quad \dot{\epsilon}_{ij}^p = \dot{\Sigma} \frac{m_{ijk} k_{ijk}}{2\Sigma}.$$ \quad (6)

For a rate independent material, Eq. (6) is valid provided that the yield condition $\Sigma = \sigma_m$ is satisfied, where $\sigma_m$ is the flow stress of the matrix material which depends on the accumulated effective plastic strain. Here, the matrix material will be assumed to obey a power law hardening function according to

$$\sigma_m = \sigma_0 \left( 1 + \frac{\dot{\Sigma}}{\dot{\epsilon}_0} \right)^N, \quad \dot{\epsilon}_p = \int \dot{\Sigma} dt,$$ \quad (7)

where $\sigma_0$ is the initial yield stress of the matrix material, $N$ is a plastic work hardening exponent and $\dot{\epsilon}_0 = \sigma_0/E_m$.

### 2.4. Interface description

The constitutive behaviour of the particle/matrix interface must satisfy the requirement of positive rate of dissipation,

$$D_I = \left( M_{ij}^I - \frac{\partial \Psi}{\partial \dot{\epsilon}_{ij}^p} \right) \dot{\epsilon}_{ij}^p \geq 0.$$ \quad (8)

Here, $\Psi$ is the free energy per unit surface area at the interface $S_I$. From a mechanical perspective in the case of proportional loading, it is immaterial whether $M_{ij}^I$ is evaluated on the basis of a purely energetic or a purely dissipative formulation (Fredriksson and Gudmundson, 2005, 2007). It should however be noted that the division between energetic and dissipative contributions is of large importance in case of elastic unloading. This case is however not considered in the present paper. Here, a purely energetic formulation will be employed and $D_I$ is taken to be zero. Regarding the specific form of $\Psi$, Asgharzadeh and Faleskog (2021a) find that it is possible to obtain precipitation strengthening in line with existing experimental results using a $\Psi$-function that depends linearly on the current value of effective plastic strain $\epsilon_{ij}^p = \sqrt{\frac{2}{3} \dot{\epsilon}_{ij}^p \dot{\epsilon}_{ij}^p}$ at the interface $S_I$. This suggests that the moment tractions can be obtained as

$$M_{ij}^I = \frac{\partial \Psi}{\partial \dot{\epsilon}_{ij}^p} = \frac{\partial \Psi}{\partial \epsilon_{ij}^p} \frac{\partial \epsilon_{ij}^p}{\partial \dot{\epsilon}_{ij}^p} = \psi' \frac{2}{3} \epsilon_{ij}.$$ \quad (9)

A convenient and appropriate definition of the proportionality factor is $\psi' = \sigma_0 \dot{\epsilon} a$, where prediction of the initial yield strength is of primary interest, cf. Asgharzadeh and Faleskog (2021a) and Faleskog and Gudmundson (2021). Here, $a$ is a non-dimensional parameter in the range $[0, 1]$ that determines the plastic constraint at an interface. As is analysed in Faleskog and Gudmundson (2021), a value of zero puts no constraint, whereas a value of one puts full constraint on the plastic strains. The latter represents a micro-hard interface where plastic strains are constrained to zero at the onset of yielding.

In the current work, post yield strain hardening is of primary interest. Therefore, the surface free energy model will be extended to account for the evolution of plastic straining. From a physical point of view, $\Psi$ should correlate with the stored energy associated with dislocation networks in the close vicinity of $S_I$.

The free energy per unit volume, $\omega$, of dislocation networks has been numerically investigated by Bertin and Cai (2018). It was found that the numerical results, for a wide range of dislocation configurations, could be very well captured by the expression

$$\omega = \frac{G_m b^2}{4\pi} \rho \ln \frac{10}{b \sqrt{\rho}}.$$ \quad (10)

This equation is based on classical analyses (see for example Hull and Bacon (2011)) for the elastic energy of a dislocation line with an effective core radius equal to 0.1b and an outer cut-off radius of $1/\sqrt{\rho}$, where $b$ denotes the magnitude of Burgers vector and $\rho$ the dislocation density. Based on Eq. (10) the energy $\Delta W$ of a volume element $\Delta V$ can be expressed as

$$\Delta W = \frac{G_m b^2}{4\pi} \Delta l \ln \frac{10d}{b}.$$ \quad (11)

where $\Delta l$ denotes the total length of dislocations in the volume element $\Delta V$ and $d = 1/\sqrt{\rho}$ represents a typical distance between dislocations.

An interface between a plastically deforming matrix material and an elastic inclusion will now be examined. Plastic deformations will then lead to an accumulation of dislocations at the interface. The surface dislocation density in this zone is denoted as $\rho$. A
surface element $\Delta A$ at the interface $S$ is now considered. The total length of dislocations in this surface element will then be $\Delta l = \hat{\rho} \Delta A$. Based on Eq. (11) the total energy $\Delta W_s$ associated with the surface element $\Delta A$ at the interface can be estimated as

$$\Delta W_s = \frac{G_m b^2}{4\pi} \Delta l \ln \frac{10d_s}{b},$$

where $d_s = 1/\hat{\rho}$ corresponds to the mean distance between the surface dislocations. Hence, the free energy per unit surface area becomes

$$\psi = \frac{\Delta W_s}{\Delta A} = \frac{G_m b^2}{4\pi} \hat{\rho} \ln \frac{10}{b d_s}.$$  \hspace{1cm} (13)

It should be noted that the influence of $d_s$ in (12) and $d_s$ in (11) may be slightly different. For simplicity, it is here assumed to be the same. Alternatively, a new constant $q$ could be introduced so that the factor 10 in (13) is replaced by $q$. For very small particles however, there may be just a few dislocations that accumulate on the surface interface. The definition of a surface dislocation density $\hat{\rho}$ may then seem inaccurate. However, if a large number of particles is considered, the total energy $\Delta W_{\text{tot}}$ for these particles can be estimated from (12) as

$$\Delta W_{\text{tot}} = \frac{G_m b^2}{4\pi} \Delta l_{\text{tot}} \ln \frac{10d_s}{b},$$

where $\Delta l_{\text{tot}}$ denotes the total length of dislocations on the collective surface elements $N \Delta A$, where $N$ is the total number of particles considered, and $d_s$ is a typical distance between dislocations. An effective surface energy density $\psi$ may then be defined as

$$\psi = \frac{\Delta W_{\text{tot}}}{N \Delta A} = \frac{G_m b^2}{4\pi N} \frac{\Delta l_{\text{tot}}}{N} \ln \frac{10d_s}{b}.$$  \hspace{1cm} (15)

Here, the surface density of dislocations can be identified as $\hat{\rho} = \Delta l_{\text{tot}}/(N \Delta A)$, and the typical distance $d_s$ can then be interpreted as $1/\hat{\rho}$. Hence, Eq. (13) is recovered.

The surface density of dislocations is related to the accumulation of plastic strain at the interface. Here, an order of magnitude argument will be presented for this relation. An interface zone of thickness $\Delta h$ and a surface area $\Delta A$ is considered. The increment of plastic strain $\varepsilon_p'$ in the interface can be estimated as

$$\varepsilon_p' \sim \frac{b \dot{A}_s}{\Delta h \Delta A}.$$  \hspace{1cm} (16)

Here, $\dot{A}_s$ denotes the increment in area swept by accumulated dislocations in the volume $\Delta A \Delta h$ of the interface zone. It can be approximately expressed as

$$\dot{A}_s \sim \hat{\rho} \Delta A \Delta h.$$  \hspace{1cm} (17)

The product $\hat{\rho} \Delta A$ denotes the increment of dislocation length resulting from accumulation of dislocations in the interface zone, and the remaining factor $\Delta h$, is an estimate of the length swept by incoming dislocations. From Eqs. (16) and (17), a linear relation between $\varepsilon_p'$ and $\hat{\rho}$ can be derived. Hence, the relation between plastic strain at the interface and surface density of dislocations can be written as

$$\hat{\rho} = \hat{\rho}_0 + \frac{k}{b} \varepsilon_p'$$

Here, $\hat{\rho}_0$ denotes the initial surface density of dislocations. The numerical constant $k$ will be of order one.

Eqs. (13) and (18) define a relation between surface energy and accumulated plastic strain at the interface. By use of Eqs. (13) and (18), and requiring that $\psi' (\varepsilon_p' = 0) = \sigma_0 \varepsilon/a$, a modified and physically based expression for $\psi'$ may after some manipulations be obtained as

$$\psi' = \sigma_0 \varepsilon/a + \omega (\varepsilon_p') = 1 - \varepsilon \ln(1 + \varepsilon_p'/\varepsilon_f).$$

Here $\varepsilon(0) = 1$ holds at the onset of overall plastic deformation, and in addition, $a \sigma_0 \varepsilon$ can be identified as $a \sigma_0 \varepsilon = G_m b k/(4\pi)$. The behaviour of function $\omega(\varepsilon_p')$ in Eq. (19) is illustrated in Fig. 2.

3. Limit analysis—Upper bound solution

Consider a volume containing a large number of elastic particles as sketched in Fig. 1 with a matrix material described by the constitutive relationships presented above. Accurate analytical solutions for initial yield stress predictions are proposed in Faleskog and Gudmundson (2021), where the authors use perturbation analysis of the governing equations on non-dimensional form to show that the plastic strain field in the matrix is to zeroth order constant for sufficiently small values of $f$ and $a/(\sigma_0 \varepsilon)$. This is exploited in Faleskog and Gudmundson (2021) to derive an upper bound solution for the initial yield stress of the composite material. The objective here is to extend the upper bound solution and develop an analytical expression in the post yield regime for the volume average stress $\langle \sigma_1 \rangle$ and how it evolves with plastic straining in the matrix. For an additional discussion of upper bound solutions for strain gradient plasticity models, see Fleck and Willis (2009b,a), Polizzotto (2010) and Reddy and Sysala (2020).
Noting that the prescribed traction $\langle \sigma_{ij} \rangle n_j$ on the external boundary to $V$ corresponds to the volume average stress, the principle of virtual work in Eq. (3) can be evaluated as

$$V(\sigma_{ij})(\epsilon^v_{ij}) = \int_V \left[ \sigma_{ij} \epsilon^v_{ij} + q_{ij} \epsilon^{vp}_{ij} + m_{ijk} \epsilon^{vp}_{ijk} \right] dV + \int_{S_I} M_{ij} \epsilon^{vp}_{ij} dS,$$

(20)

where $\langle \epsilon^v_{ij} \rangle$ is the volume average virtual strain resulting from the arbitrary virtual displacements $u^*_i$ and $\epsilon^v_{ij} = \epsilon^*_{ij} - \epsilon^v_{ij}$, where $\epsilon^v_{ij}$ is independent of $\epsilon^*_i$ according to (20). Note that it is assumed that the moment tractions vanish at the external boundary.

The principle of maximum plastic dissipation, cf. Eq. (4), may now be formulated by the following inequality

$$q_{ij} \epsilon^v_{ij} + m_{ijk} \epsilon^{vp}_{ijk} \leq q^*_i \epsilon^v_{ij} + m^*_{ijk} \epsilon^{vp}_{ijk} = \sigma_m E^p.$$

(21)

Here, $q^*_i$ and $m^*_{ijk}$ are the micro stresses and moment stresses corresponding to $\epsilon^v_{ij}$ and $\epsilon^{vp}_{ij}$, respectively, according to Eq. (6), and $E^p$ is the virtual effective plastic strain. Utilizing constitutive relation (9) for $M_{ij}$ at the interface, the following inequality apply for the last term in Eq. (20),

$$M_{ij} \epsilon^{vp}_{ij} = \psi \frac{2}{3} \frac{E^p}{\sqrt{\pi}} \frac{\epsilon^{vp}_{ij} \epsilon^{vp}_{ij}}{\epsilon^v_{ij}} \leq \psi \frac{2}{3} \frac{\epsilon^{vp}_{ij} \epsilon^{vp}_{ij}}{\epsilon^v_{ij}} = \psi \epsilon^p.$$

(22)

An inequality may now be formulated from Eqs. (20)–(22) for the volume average stress,

$$V(\sigma_{ij})(\epsilon^v_{ij}) \leq \int_V \sigma_{ij} \epsilon^v_{ij} dV + \int_V \left[ \sigma_{ij} \epsilon^v_{ij} + \sigma_m E^p \right] dV + \int_{S_i} \psi \epsilon^p dS,$$

(23)

where the integration over $V$ has been split up into sub-volumes $V_p$ and $V_m$.

Based on the perturbation analysis in Faleskog and Gudmundson (2021) assuming sufficiently small $a/\varepsilon$ and $f$, a homogeneous virtual strain field $\varepsilon^v_{ij}$ corresponding to virtual displacements $u^*_i = \varepsilon^v_{ij} x_j$, will be assumed in the present analysis. Thus, in the elastic particles residing in $V_p$, $\varepsilon^v_{ij} = \varepsilon^0_{ij}$. In the matrix $V_m$, it will be assumed that $\varepsilon^v_{ij} = \varepsilon^p_{ij}$ and $\varepsilon^v_{ij} = 0$. With these assumptions, (23) may be evaluated as

$$\left[ (\sigma_{ij})_p - f \langle \sigma_{ij} \rangle_p \right] \frac{\varepsilon^0_{ij}}{\varepsilon^v_{ij}} \leq (1-f) \sigma_m + \frac{1}{V} \int_{S_i} \psi \varepsilon^p dS,$$

(24)

where $\varepsilon^0_{ij}$ is the effective plastic strain corresponding to $\varepsilon^0_{ij}$ and thus $E^p = \varepsilon^0_{ij}$, and $\sigma_m$ represents the flow stress of the matrix in absence of strain gradients. Furthermore, $\langle \sigma_{ij} \rangle_p$ denotes the volume average stress in all the particles, and $f = V_p/V$ is the total volume fraction of particles. Uniformity of plastic strain has also been used as a basis in the theory of Brown and Stobbs (1971) and has moreover been argued for by Mura (1987). In situations where the plastic deformation is accommodated by the formation of dislocation shear bands, or other localization phenomena, this assumption can of course not be valid.

It is noted that the inequality in Eq. (24) only depends on the direction of $\varepsilon^0_{ij}$ and not on its magnitude. Moreover, since the virtual strains are volume preserving, only the deviatoric parts $\langle s_{ij} \rangle$ and $\langle s_{ij} \rangle_p$ of $\langle \sigma_{ij} \rangle$ and $\langle \sigma_{ij} \rangle_p$, respectively, will contribute to Eq. (24). Hence,

$$\left[ (s_{ij})_p - f \langle s_{ij} \rangle_p \right] \frac{\varepsilon^0_{ij}}{\varepsilon^v_{ij}} \leq (1-f) \sigma_m + \frac{1}{V} \int_{S_i} \psi \varepsilon^p dS.$$

(25)

The right-hand-side of Eq. (25) does not depend on either the applied stress nor on the assumed virtual strain $\varepsilon^0_{ij}$. To obtain the lowest possible bound for the external loading, the left-hand-side of Eq. (25) should be maximized for a given $\langle s_{ij} \rangle$. This is achieved...
when \( \epsilon_i^0 \) is co-linear with \( \langle s_{ij} \rangle - f(s_{ij}) \). Furthermore, the average stress deviator in particles is related to the applied deviatoric stress and the plastic strain evolving in the matrix in the post yield regime. This relation can be established by introducing a known eigenstrain in the particles that reflects the homogeneous plastic strain in the matrix, and analysing the composite as an Eshelby problem, cf. Eshelby (1957) and Mura (1987). Details of this analysis is given in Appendix, and for particles of spherical shape this relation can be expressed as

\[
\langle s_{ij} \rangle_p = \tilde{F} \langle s_{ij} \rangle + 2\tilde{G} \epsilon_i^p,
\]

(26)

where \( \tilde{F} \) and \( \tilde{G} \) represent effective values of \( F \) and \( G \) for the composite in case the elastic properties differ among particles, and \( \epsilon_i^p \) denotes the homogeneous plastic strain assumed to prevail in the matrix, i.e. in volume \( V_m = (1-f)V \). For an individual spherical particle (see Appendix)

\[
F = \frac{15(1-v_m)g}{7 - 5v_m + 2(4-5v_m)g} = 3v_m = 0.3 = \frac{21g}{11 + 10g},
\]

(27)

\[
G = \frac{15(1-v_m)g}{7 - 5v_m + 2(4-5v_m)g} = 3v_m = 0.3 = \frac{11G_{m}g}{11 + 10g},
\]

where \( g = G_p/G_m \). It is noteworthy that \( G/(FG_m) = (7 - 5v_m)/(15(1 - v_m)) \), i.e. this ratio is independent of \( g \) and only exhibits a weak dependence on \( v_m \).

By applying a virtual strain field \( \epsilon_i^v \) that is co-linear with \( \langle s_{ij} \rangle - f(s_{ij}) \), the left-hand-side of Eq. (25) may be simplified as

\[
\sqrt{\frac{3}{2}} \left( \langle s_{ij} \rangle - f(s_{ij}) \right) \left( \langle s_{ij} \rangle - f(s_{ij}) \right)^\prime = \sqrt{\left( \langle \sigma_c \rangle(1 - f \tilde{F}) \right)^2 - 2(1 - f \tilde{F}) \langle \sigma_c \rangle G \sigma_i^p + (3\tilde{G}f \epsilon_i^p)^2} = \sigma_c (1 - f \tilde{F}) - 3\tilde{G}f \epsilon_i^p.
\]

(28)

To arrive at the second step in Eq. (28), equalities \( 3\langle s_{ij} \rangle/2 = \langle \sigma_i^e \rangle, \epsilon_i^p \epsilon_i^p = 3(\epsilon_i^p)^2/2 \) and \( \langle s_{ij} \rangle \epsilon_i^p = \langle \sigma_c \rangle \epsilon_i^p \) have been utilized. The latter equality rests on the assumption of proportional loading, which is justified in this case. Also, the bracket symbol \( (\cdot) \) has been omitted in the third step in Eq. (28) and will henceforth not be used.

Returning to Eq. (25), the second term on the right-hand-side may for spherical particles be evaluated as

\[
\frac{1}{V} \int_{S_1} \psi \, dS' = 3f \sigma_c \tilde{a} \tilde{\omega} \frac{\tilde{\epsilon}}{\tilde{a}},
\]

(29)

where \( \tilde{a} \) and \( a \) represent effective values of \( a \) and \( a \), respectively, which will be defined below.

Finally, by substitution of Eqs. (28) and (29) into (25), the upper bound solution for the effective stress (flow stress) of a composite containing a random distribution of elastic spherical particles can be formulated as

\[
\sigma_c \leq \frac{(1 - f)}{(1 - f \tilde{F})} \sigma_m(\epsilon_c^p) + \frac{3f \sigma_c \tilde{a} \tilde{\omega} \alpha (\epsilon_i^p)}{(1 - f \tilde{F})} \tilde{a} + \frac{3\tilde{G}f}{(1 - f \tilde{F})} \epsilon_i^p = \sigma_c^{UBS},
\]

(30)

where

\[
\epsilon_c^p = \frac{\tilde{\epsilon}_c^p}{1 - f}.
\]

(31)

Here, \( \tilde{\epsilon}_c^p \) denotes the volume average of the effective plastic strain in the composite material in \( V \). This is a more convenient measure for practical purposes, and will be used in Section 4 where model predictions are compared with full field FEM results. Note that the first term in Eq. (30) is the flow stress from the matrix material adjusted for a volume fraction of particles and that the second and third term correspond to particles’ contributions to yield stress and strain hardening, respectively. Also, notice that the third term in Eq. (30) corresponds to a particle induced linear strain hardening, similar to what has been derived in Tanaka and Mori (1970) and Brown and Stobbs (1971). However, the linear hardening may be counteracted by the second term in Eq. (30) if the interface suffers from a logarithmic decay with increasing effective plastic strain.

The effective values in Eq. (30) are evaluated as

\[
\tilde{F} = \frac{(\Gamma \sigma \langle a^3 \rangle)}{(a^3)}, \quad \tilde{G} = \frac{(G\sigma \langle a^3 \rangle)}{(a^3)}, \quad \tilde{\omega} = \frac{(\alpha \langle a^3 \rangle)}{(a^3)}, \quad \tilde{a} = \frac{(\langle a^3 \rangle)}{(a^3)},
\]

(32)

where \( \langle a \rangle = \frac{\sum_{n=1}^{N_p} a_i}{N_p} \) denotes the mean value taken over all \( N_p \) particles in \( V \). Notice that only the interface parameter \( \alpha \) is subject to averaging whereas the parameters associated with the non-dimensional function \( \omega \) are assumed to belong to the matrix material. If all particles possess the same properties, the effective properties in Eq. (32) simplify to

\[
\tilde{F} = F, \quad \tilde{G} = G, \quad \tilde{\omega} = \alpha = a.
\]

(33)

Moreover, if all particles have the same size, \( \tilde{a} = a \).

4. Numerical validation of upper bound solution

A numerical examination and validation of the upper bound solution (UBS) extended for post yield strain hardening will now be presented. For this purpose, two different unit cell models will be employed, where full-field solutions are obtained by finite element analysis. General model features and overall accuracy will be discussed first on the basis of a 2D-axisymmetric model, where both perfectly plastic and strain hardening matrix materials are considered, with or without a decaying interface strength. This is followed by three-dimensional analyses, where variations of interface strength and shear modulus with particle size are investigated in the post yield regime.
boundary conditions were enforced as referenced above. Solver and OpenMP parallelization were utilized to speed up the computations. For details the reader is referred to the papers. The algorithm was used to establish the linearized equation system, which was solved in an iterative manner in the FEM code. A sparse discussion on appropriate values for the current application, see Asgharzadeh and Faleskog (2021a). Furthermore, an Euler-backward to rate independent results can effectively be achieved provided that \( \alpha \) is chosen to follow a geometric series such that the surface area ratio between the largest and smallest particle becomes 10. Thus, \( \alpha = \alpha_1 \lambda^{i-1} \) with \( \lambda = 10^{1/14} \), where \( \alpha_1 \) is determined by the volume fraction \( f \) as \( \alpha_1 = H \left[ 48 f (\lambda^3 - 1) / (\sigma_0 \lambda^{24} - 1) \right]^{1/4} \).

These unit cell models have proven to be suitable for numerical validation of the upper bound model for yield stress predictions (cf. Faleskog and Gudmundson, 2021). The numerical analysis performed in the present study utilizes the FEM formulation developed for plane strain in Dahlberg and Faleskog (2013) and Dahlberg et al. (2013), and the extension to axisymmetry in Asgharzadeh and Faleskog (2021a). The corresponding 3D formulation is given in Asgharzadeh and Faleskog (2021b). The in-house FEM code was further developed in this work by implementation of a hexahedral 20 node element with an associated 16 node interface element.

Both particles and the matrix material were discretized by use of the same type of elements and thus modelled as SGP materials. Elastic conditions in particles were enforced by prescribing \( \varepsilon \) for 2D axisymmetry, and in Asgharzadeh and Faleskog (2021b) for 3D. As \( \varepsilon \) was prescribed in all particles, reaction traction moments will arise at nodes with plastic dof in an interface element facing a particle.

A typical cubic mesh is shown in Fig. 4, where also the hexahedral and 3D interface elements are illustrated. In an element, displacements and plastic strains are described using tri-quadratic and tri-linear interpolations, respectively. Thus, all primary moments will arise at nodes with plastic dof in an interface element facing a particle.

To circumvent the problem of the indeterminacy of \( q_{ij}, m_{ijk} \) in the elastic regime, the rate dependent visco-plastic constitutive formulation proposed in Dahlberg and Faleskog (2013) was used. Specifically, the effective plastic strain rate \( \dot{\varepsilon} \) in Eqs. (4)–(7) is governed by a viscosity law \( \dot{\varepsilon} = \dot{\varepsilon}_0 \Phi(\Sigma, \sigma_m) \), where \( \Phi(\Sigma, \sigma_m) = \kappa(\Sigma / \sigma_m) + (\Sigma / \sigma_m)^n \) (visco-plastic response function). However, close to rate independent results can effectively be achieved provided that \( \kappa \) and \( n \) are small respectively large. For a detailed discussion on appropriate values for the current application, see Asgharzadeh and Faleskog (2021a). Furthermore, an Euler-backward algorithm was used to establish the linearized equation system, which was solved in an iterative manner in the FEM code. A sparse solver and OpenMP parallelization were utilized to speed up the computations. For details the reader is referred to the papers referenced above.

Symmetry displacement boundary conditions were applied on the unit cells in a standard manner. The higher order symmetric boundary conditions were enforced as

**3D-cubic:**
\[
\begin{align*}
M_{xx} &= M_{yy} = M_{zz} = M_{xy} = 0, \\
\varepsilon_{xx} &= \varepsilon_{yy} = \varepsilon_{zz} = 0 \\
\end{align*}
\]
\( \text{on } x = 0 \text{ and } x = H \)
\[
\begin{align*}
M_{xx} &= M_{yy} = M_{zz} = M_{xz} = 0, \\
\varepsilon_{xx} &= \varepsilon_{yy} = \varepsilon_{zz} = 0 \\
\end{align*}
\]
\( \text{on } y = 0 \text{ and } y = H \)
\[
\begin{align*}
M_{xx} &= M_{yy} = M_{zz} = M_{xy} = 0, \\
\varepsilon_{xx} &= \varepsilon_{yy} = \varepsilon_{zz} = 0 \\
\end{align*}
\]
\( \text{on } z = 0 \text{ and } z = H \)

**2D-axisymmetric:**
\[
\begin{align*}
M_{rr} &= M_{zz} = 0, \\
\varepsilon_{rr} &= \varepsilon_{zz} = 0 \\
\end{align*}
\]
\( \text{on } r = 0, R \text{ and } z = 0, H \)
As the flow stress in Eq. (30) only depends on the second deviatoric stress invariant, it suffices to analyse uniaxial tension. Thus, all unit cells were subjected to loading in uniaxial tension which, together with the symmetry boundary conditions, was applied by use of Lagrange equations.

The volume average of the Cauchy stress and its effective value in a unit cell were calculated as

$$\bar{\sigma}_{ij} = \frac{1}{V} \int_{S_{ext}} \frac{1}{2} (\sigma_{ik} x_k n_i + \sigma_{jk} x_j n_k) \, dS, \quad \bar{\sigma}_e = \sqrt{\frac{3}{2} \bar{\sigma}_{ij} \bar{\sigma}_{ij},}$$

and the volume average of strain and the effective strain were evaluated as

$$\bar{\epsilon}_{ij} = \frac{1}{V} \int_{S_{ext}} \frac{1}{2} (u_i n_j + u_j n_i) \, dS, \quad \bar{\epsilon}_e = \sqrt{\frac{3}{2} \bar{\epsilon}_{ij} \bar{\epsilon}_{ij},}$$

The results from the unit cell analyses presented below will be referred to as ‘FEM’ if obtained by finite element analysis or as ‘UBS’ if obtained by the upper bound solution (Eq. (30)). Key parameters in the analysis are \( f \), \( \ell / \bar{a} \), and the ratio between the shear modulus in particles and matrix, respectively, as this ratio enters in parameters \( \bar{\gamma} \) and \( \bar{G} \). Poisson’s ratio play a minor role, and \( \nu_p = \nu_m = 0.3 \) will be used throughout the analysis.

Below, the upper bound solution will be compared with the outcome from numerical analyses of the unit cell models. Volume average effective stress–strain curves may then be constructed for the upper bound solution as

$$\sigma_e = \begin{cases} 3G_{eff} \bar{\epsilon}_e, & \bar{\epsilon}_e \leq \epsilon_{y0} \\ \sigma_{UBS}^{eff} \bar{\epsilon}_e, & \bar{\epsilon}_e > \epsilon_{y0} \end{cases} \quad \text{where} \quad \bar{\epsilon}_e = 3G_{eff}^{UBS} (\bar{\epsilon}_e^p / 3G_{eff}^{UBS} + \bar{\epsilon}_e^p).$$

Here, \( \epsilon_{y0} = \sigma_{y0} \) represents the strain at the onset of overall plastic deformation with \( \sigma_{y0} = \sigma_{UBS}^{eff}(0) \) being the yield stress, and \( G_{eff}^{UBS} \) is the effective shear modulus of the composite material. The latter may be determined by use of Eshelby’s equivalent inclusion method, which for spherical particles become (see pp. 428–430 in Mura (1987))

$$G_{eff} = \frac{G_m}{1 + f \bar{\gamma}},$$

where

$$\bar{\gamma} = \frac{(\gamma a^3)}{(a^1)} \quad \text{with} \quad \gamma = \frac{15(1 - \nu_m)(1 - g)}{7 - 5\nu_m + 2(4 - 5\nu_m)g}. \quad (39)$$

The tangent modulus of the effective stress–strain curve (37) will be compared with that obtained from unit cell analysis. For a perfectly plastic matrix combined with an interface energy independent of plastic straining, the tangent modulus takes the simple form

$$\frac{d\sigma_e}{d\bar{\epsilon}_e} = \frac{h_{UBS}}{1 + h_{UBS}/3G_{eff}} \quad \text{with} \quad h_{UBS} = \frac{3\bar{G} f}{(1 - f)(1 - f)}.$$

4.2. Strain hardening and hardening saturation: A perfectly plastic matrix

The upper bound solution (Eq. (30)) show that the flow stress depends on the size distribution of particles through the effective value \( \bar{a} \), and also through \( \bar{a}, \bar{\gamma} \) and \( \bar{G} \) if their interface properties respectively shear modulus vary with particle size. To demonstrate this, numerical results were generated by use of the 2D axisymmetric model with three different cell ratios, \( H/R = 0.5, 1.2, \) and
Fig. 5. A material with a perfectly plastic matrix material reinforced by a 2% volume fraction of particles with interface strength $\alpha = 0.99$ and relative size $\bar{a}/\ell = 1/16.498$. Normalized volume average effective stress–strain curves for different particle arrangements; (a) linear regime I and (b) saturation regime II. (c) Effective plastic strain plotted versus radius at $z = 0$ resulting from the 2D axisymmetric model with $H = R$.

use of the 3D cube model containing particles with the size variation described in Section 4.1. A material with a perfectly plastic matrix ($N = 0$) containing particles with the same shear modulus as the matrix ($G = 1$), a volume fraction $f = 0.02$, and an almost micro-hard particle/matrix interface $\alpha = 0.99$ with $\omega = 1$ ($c = 0$), was considered. In addition, a ratio $\ell/\bar{a} = 16.498$ was chosen, which according to Eq. (30) gives an initial yield stress $\sigma_{y0} = 2\sigma_0$. The resulting overall effective stress–strain curves are shown in Fig. 5(a). The curves are normalized by $\sigma_0$ and $\varepsilon_{y0}$, respectively. As noted, the results from the unit cell analyses coincide and are well captured by the UBS (curve in colour red).

As the applied strain increases and becomes sufficiently large, the numerical results reveal that the UBS ceases to be valid, see region II in Fig. 5(b). At this instance in the loading, the stress saturates (recall that the matrix is perfectly plastic, i.e. no hardening is provided by the matrix) and particles no longer contribute with additional strain hardening. The transition from linear hardening to zero hardening occurs at a strain that seems to scale with $\varepsilon_{y0}/\ell/\bar{a} \cdot (1 + 1/G)$ and also depends on the spatial arrangement of particles as can be concluded from the spread in results noticed in region II in Fig. 5(b). This will be further elaborated on in Section 4.6.

Some insight to this phenomenon can be gained by the characteristics of the distribution of effective plastic strain $\varepsilon_p^e$ in the matrix material at increasing levels of the overall strain. Radial distributions of $\varepsilon_p^e$ at $z = 0$ obtained from the axisymmetric analysis with $H = R$ are presented in Fig. 5(c). At sufficiently low strain levels (curve labelled 3), it is noted that $\varepsilon_p^e$ is essentially homogeneous in the matrix material. This agrees with the analytical predictions for $a/\ell \ll 1$ presented in Faleskog and Gudmundson (2021). However, as the overall strain increases, a noticeable strain gradient develops near the interface of the particle (curves labelled...
4 and 5). Eventually the interface becomes incrementally micro-hard, and further development of plastic strain at the interface vanishes, which leads to even stronger plastic strain gradients in the matrix (curves labelled 6 to 8). At this stage in the loading, the overall stress level saturates.

Nevertheless, the UBS appears to be valid up to rather large strain levels (region I) as noted in the examples shown in Fig. 5(b). This suggests that the proposed UBS may be used for quite a wide range of physically relevant model parameters.

### 4.3. Assessment of post yield response of the upper bound solution

A selective parametric study will now be presented based on the 2D axisymmetric model to explore the influence of the volume fraction \( f \), modulus mismatch \( g = G_p/G_m \), matrix strain hardening \( N \), and the interface strength decay coefficients \( \epsilon \) and \( \epsilon_f \), on strain hardening and the accuracy of UBS predictions. In all cases the ratio \( \epsilon / \dot{\epsilon} \) was chosen such that \( \epsilon_{UBS}^{UBS} (0) = 2 \sigma_0 \) in a microstructure with a medium strong particle/matrix interface \( \alpha = 0.5 \). All FEM calculations were progressed until an effective strain \( \dot{\epsilon} = 11 \varepsilon_{\text{y0}} \) was reached.

Particles with an interface strength \( \psi' \) that is independent on plastic strain (\( \epsilon = 0 \) in (19)) and embedded in a perfectly plastic matrix (\( N = 0 \)) are considered first. Fig. 6(a) shows effective stress–strain responses for \( f = (0.02, 0.04, 0.08) \) with \( G_p = G_m \). Solid lines pertain to UBS predictions and dashed lines to FEM results. As observed, the UBS predictions agree very well with the FEM results, but some deviation is noticed for the material with the highest volume fraction (\( f = 0.08 \)). This trend may be expected, as the accuracy of the UBS is closely related to the accuracy of the Eshelby solution, which assumes that particles are remote from each other. The effects of a mismatch in shear modulus are shown in Fig. 6(b) for materials with \( G_p/G_m = (0.1, 1, 10) \), all having \( f = 0.02 \). Again, the agreement between the UBS predictions and FEM results are very good.

Now, the perfectly plastic matrix is exchanged with a strain hardening matrix. The interaction between a strain hardening matrix and hardening due to particles is displayed in Fig. 6(c). Here, stress–strain curves for materials with hardening exponents \( N = (0, 0.1, 0.2) \), with \( f = 0.02 \) and \( G_p = G_m \) are shown. As noticed, the UBS predictions fully captures the stress–strain curves resulting from the FEM analysis.

If the interface suffers from a logarithmic decay evolving with plastic straining, softening may follow upon the onset of overall plastic yielding. The degree of softening depends on the interplay between matrix strain hardening with additional contribution from particles, and the interface decay governed by parameters \( \epsilon \) and \( \epsilon_f \) (illustrated in Fig. 2).

Thus, softening is most pronounced in materials with a perfectly plastic matrix (\( N = 0 \)), as can be observed from the examples shown in Fig. 7(a). Here, stress–strain curves are plotted for three different interfaces: \( \epsilon = (0.15, 0.3) \) with \( \epsilon_f = 0.88\sigma_0/3G_m \) and volume fraction \( f = 0.02 \) of particles with matching shear modulus \( (G_p = G_m) \). The ensuing softening is significant, and here, the linear hardening contribution from particles observed for \( c = 0 \) is completely wiped out by the decaying interface strength, as seen by the curves with \( c > 0 \).

The interplay between matrix strain hardening and interface decay is shown in Fig. 7(b). This graph shows four stress–strain curves, which were generated by combinations of \( N = (0.1, 0.2) \) and \( \epsilon = (0.15, 0.3) \) with \( \epsilon_f = 0.88\sigma_0/3G_m \). Particles have volume fraction \( f = 0.02 \) and a shear modulus \( G_p = 5G_m \). In these examples, only materials with \( N = 0.1 \) exhibit some initial softening at onset of plastic deformation. It is noteworthy that all UBS predictions virtually lie on top of the FEM results in Fig. 7.

### 4.4. Overall accuracy of the upper bound solution

The volume fraction of particles \( f \) and the shear modulus ratio \( G_p/G_m \) play key roles for the flow properties of the composite according to Eq. (30), as both affect initial yield stress and strain hardening. In addition, the yield stress is strongly affected by the ratio \( \epsilon / \dot{\epsilon} \). In Faleskog and Gudmundson (2021) it is suggested that intervals of practical relevance for these parameters are \( 0.001 \leq f \leq 0.1 \), \( 1 \leq \epsilon / \dot{\epsilon} \leq 100 \) and \( 0.1 \leq G_p/G_m \leq 10 \), where error maps for UBS predictions of yield stress are presented. Here, an analogous FEM analysis was carried out by use of the 2D axisymmetric model to investigate the accuracy of UBS predictions well into the post yield regime. This is accomplished by loading the unit cell until an effective strain \( \dot{\epsilon}_{\varepsilon_{\text{y}}} \), defined where \( \dot{\varepsilon}_{\varepsilon_{\text{y}}} = 10\varepsilon_{\text{y0}} \) in (37), was reached. Calculations were performed on materials with a medium strong interface (\( \alpha = 0.5 \)) and a micro-hard interface (\( \alpha = 1 \)), both with \( \omega = 1 \). Three modulus mismatch ratios were considered; an under-matched \( G_p = 0.1G_m \), a matched \( G_p = G_m \), and an over-matched \( G_p = 10G_m \), respectively.

The accuracy of the UBS predictions is presented in Fig. 8 as iso-contours of the relative error (in percent) of the UBS predictions, which are plotted in \( \epsilon / \dot{\epsilon} \) versus \( f \) graphs on log–log scale. Thus, the relative error is defined as \( [\sigma_{UBS}/\sigma_{FEM} - 1] \times 100 \), which was evaluated at \( \dot{\varepsilon}_{\varepsilon_{\text{y}}} = \dot{\varepsilon}_{\varepsilon_{\text{y}}} \). Error maps for material systems with \( \alpha = 0.5 \) are shown in Figs. 8(a)–(c). As can be seen, the accuracy of the UBS predictions is within \( \pm 1\% \) for materials over a broad range in the parameter space, especially for under-matched systems with \( G_p < G_m \). For matched and over-matched systems (\( G_p \geq G_m \)), the accuracy of UBS predictions is somewhat impaired at lower ratios of \( \epsilon / \dot{\epsilon} \) when \( \varepsilon \) becomes high. The trends are the same for materials with micro-hard interfaces as noted in Figs. 8(d)–(f), although the regions in which the relative error is within \( \pm 1\% \) are slightly reduced. Insight into the decreasing accuracy noticed in regions with lower ratios of \( \epsilon / \dot{\epsilon} \) in Fig. 8 may be understood from the observation made in Fig. 5. Even if the UBS is highly accurate at the onset of plastic yielding, as also noted in Faleskog and Gudmundson (2021), it will cease to be valid at sufficiently high strain levels where the particle induced strain hardening saturates, as seen in Fig. 5. The strain level marking the transition to saturation depends on \( \epsilon / \dot{\epsilon} \) and \( G_p/G_m \) as discussed above and further elaborated on in Section 4.6. The possible impact of this phenomenon on the error maps in Fig. 8 can be ascertained by plotting the hardening slope evaluated at \( \dot{\varepsilon}_{\varepsilon_{\text{y}}} = \dot{\varepsilon}_{\varepsilon_{\text{y}}} \), from FEM calculations, \( d\dot{\varepsilon}_{\varepsilon_{\text{y}}} \), normalized by the linear hardening slope obtained from UBS according to Eq. (40). If this quotient becomes significantly smaller than one, the hardening has begun to saturate. The regions with a relative error significantly larger than the one seen in Fig. 8 are indeed associated with a quotient much less than one, as can be concluded from Fig. 9, where this quotient is plotted.
4.5. 3D-Validation: Variation of interface strength and shear modulus with particle size

So far, materials with monodisperse particle distributions have been analysed, but particles in real materials typically exhibit some variation in size. This aspect was addressed by use of the 3D cube model in Fig. 3(b). It was assumed that particles varied according to a geometric series as described in Section 4.1, with a ratio between the largest and smallest radius of \(a_8/a_1 = 3.16\). Hence, the variation in particle size is significant, and the effective particle radius is according to Eq. (32), \(\bar{a} = 2.405a_1\) (the geometric mean value is \(1.907a_1\)). Two sets of analyses were carried out. In the first set, the interface strength depends on particle size, whereas the shear modulus does not. In the second set, the interface strength is independent on particle size and the shear modulus vary with particle size.

In the first set, a linear variation of interface strength with particle size was considered, defined as \(\alpha_i = \alpha_1[1-(a_i-a_1)/a_8]\), where \(\alpha_1 = 0.98\). Moreover, interfaces were assumed to be independent on the accumulated plastic strain (\(\omega = 1\)). The effective interface strength of the composite is then given by Eq. (32) as \(\bar{\alpha} = 0.545\). Results from the first set are shown in Fig. 10, where effective stress–strain curves from UBS (Eqs. (30)–(32),(37)) are compared with the outcome from the FEM analyses. Three graphs are presented, pertaining to \(f = 0.02, 0.04, 0.08\). In each graph, three different shear moduli are considered for the particles: \(G_p/G_m = [0.2, 1, 5]\). As noticed, the model predictions agree very well with the FEM results for the lower \(f\) values, but at the highest volume fraction of particles (\(f = 0.08\)), some deviations are noticed for stiff particles (\(G_p = 5G_m\)).
Fig. 7. Comparison of normalized volume average effective stress–strain curves resulting from UBS and FEM analysis of the 2D axisymmetric model, for a variation of the decay parameter $c$ in an initially strong interface ($\alpha = 0.99$). (a) A material with perfectly plastic matrix and particles with $G_p = G_m$. (b) Materials with strain hardening matrix, $N = [0.1, 0.2]$, and particles with $G_p = 5G_m$. In both (a) and (b) the volume fraction of particles equals 2%.

Fig. 8. Error maps showing relative error in percent defined as $(\bar{\sigma}_{\text{FEM}}/\bar{\sigma}_{\text{UBS}} - 1) \times 100$ plotted in $f$ versus $\ell/a$ graphs on log–log scale. In graphs (a)–(c), $\alpha = 0.5$ and in graphs (d)–(f), $\alpha = 1$. The first, second and third column belongs to $G_p/G_m = 0.1, 1$ and 10, respectively.
Fig. 9. Ratio of the volume average effective stress–strain tangent between FEM and UBS, obtained at $\dot{\varepsilon}_p = \varepsilon_{p*}$, plotted in $f$ versus $\ell/a$ graphs on log–log scale. In graphs (a)–(c), $\alpha = 0.5$ and in graphs (d)–(f), $\alpha = 1$. The first, second and third column belongs to $G_p/G_m = 0.1, 1$ and 10, respectively.

In the second set, the interface strength of all particles was chosen to be equal to the effective value resulting in set 1, i.e. $\alpha = 0.545$, and the shear modulus was taken to vary linearly with particle size as $G_p = (1 - \xi_i)G_{p1} + \xi_i G_{p8}$, where $\xi_i = (a_i - a_1)/(a_8 - a_1)$. Ratios $G_{p1}/G_{p8}$ equal to $1/4$, $1/2$, 2 and 4 were considered, and the relation to the matrix shear modulus was chosen such that $\bar{\gamma} = 1$ by use of Eqs. (27) and (32). As both $\bar{\gamma}$ and $\bar{\gamma}$ are evaluated in the same manner, cf. Eq. (32), both strengthening and strain hardening are expected to be independent of ratio $G_{p1}/G_{p8}$ under this circumstance, and only depend on $f$. Moreover, with $\bar{\gamma} = 1$, Eq. (38) gives that $G_{eff} = G_m$. The results can be observed in Fig. 11, where effective stress–strain curves are plotted for volume fractions $f = 0.02, 0.04, 0.08$, and clearly show hardening slopes independent of $G_{p1}/G_{p8}$. Note that each $f$ value is represented by four curves pertaining to UBS and four curves belonging to the FEM analysis, and that all curves collapse on top of each other.

4.6. Saturation of particle induced strain hardening

The results shown in Fig. 5(a) strongly suggest that the additional hardening due to particles that remains elastic will saturate at a certain level of overall plastic straining. This hardening behaviour is in line with what is commonly observed in alloys containing hard second phase particles, e.g. Fribourg et al. (2011), Lloyd (1994), Myhr et al. (2010) and Fazeli et al. (2008a). Qualitatively, it resembles stages II and III in classic work hardening theory for polycrystals.

As is noteworthy, the saturation of stress observed in Fig. 5(b) is also followed by a saturation of plastic strain at the particle/matrix interface, see Fig. 5(c). Physically, this can be tied to the process of plastic relaxation, by which, the accumulation rate of dislocations surrounding particles is reduced, see e.g. Myhr et al. (2010) and Fribourg et al. (2011). The transition from linear hardening to saturation will here be addressed in a purely phenomenological manner. As such, the following function is introduced:

$$\phi_T = \left(1 + \left(\frac{\varepsilon_p}{\varepsilon_T}\right)^q\right)^{-1/q}.$$  

(41)

In Eq. (41), $\varepsilon_T$ corresponds to the intersection between the linear slope in region I, Eqs. (30)–(31), and a numerical estimate of the saturation stress level $\sigma_\infty$ (see Fig. 5(b)). Moreover, $q$ is an exponent in the range 2 to 4. The relevance of this function can be seen in Fig. 12, where a comparison is made between Eq. (41) and the results from a large amount of numerical simulations using the
Fig. 10. Comparison of normalized volume average effective stress–strain curves resulting from UBS and FEM analysis of the 3D cubic model, for materials with a perfectly plastic matrix and interfaces with linearly varying strength \( \alpha = 0.98, \ldots, \alpha = 0.31 \). Particle volume fractions: (a) 2%, (b) 4%, and (c) 8%.

axi-symmetric model with an isotropic distribution of particles of radius \( a \). Using the simulation results underpinning Fig. 12, it is also possible to find an explicit expression for \( \varepsilon_T \) on the following form:

\[
\varepsilon_T \approx K \varepsilon_0 \frac{f}{a} (1 + \frac{G_m}{G_p}),
\]

where \( \varepsilon_0 = \sigma_0 / E_m \) refers to the yield strain of the matrix material. For spherical particles distributed as shown in Fig. 3(a) with \( H = R, K \approx 15 \). Note that the simple relation (42) is qualitatively supported by the trend observed in Fig. 9, where the decrease in the tangent of the effective stress–strain curves obtained from FEM seems to scale with \( f/a \) with a negligible influence of \( f \). Furthermore, in Faleskog and Gudmundson (2021), a perturbation analysis based on a non-dimensional form of the governing equations (2)–(19) was carried out. The analysis was based on the assumption of \( f \ll 1 \) and \( a/f \ll 1 \), following the notation in the present paper. A closed form solution for the initial yield stress was in this way possible to derive. If the corresponding analysis is extended to strain hardening, it can be concluded that the perturbation assumptions break down for a plastic strain of the order of \( \varepsilon_0 \varepsilon / a \). This is confirmed by the estimate expressed in Eq. (42).

5. Strengthening contribution from particles subjected to shearing

The strengthening mechanism addressed so far is associated with dislocations that by-pass particles at the onset of macroscopic plastic straining. However, if the size of a particle located on a slip plane is sufficiently small it will be sheared by dislocations
Fig. 11. Comparison of normalized volume average effective stress–strain curves resulting from UBS and FEM analysis of the 3D cubic model, for \( f = \{0.02, 0.04, 0.08\} \). The matrix is perfectly plastic and the shear modulus of the particles vary with their size.

Fig. 12. Normalized strain hardening plotted vs. effective plastic strain normalized the transition strain introduced in Eq. (41). Dashed lines in colour red represents Eq. (41) evaluated for \( q = 2, 3, 4 \).

instead. In general, this shearing mechanism will primarily affect the yield strength of the material. The obstacle strength from a sheared particle depends on size in some manner, and several models have been proposed for this dependency, see discussions in Ardell (1985) and Reppich (1993). To account for this additional strength contribution, the model proposed in Deschamps and Brechet (1998) will be employed and incorporated into the upper bound solution.

A distribution of particle size may be represented by a discrete or continuous random variable described by some appropriate distribution function. Assume that particles will be sheared if belonging to a population of \( N_s \) particles with a radius less than or equal to \( a_c \). The remaining particles will be by-passed by dislocations and belong to a population of \( N_b \) particles. The total number of particles in \( V \) is then \( N_p = N_s + N_b \).

In Deschamps and Brechet (1998), it is assumed that the obstacle strength of a sheared particle depends linearly on the particle size. The contribution to strengthening then hinges on assumptions made for mean particle spacing, which in turn depends on obstacle strength. Three models for the contribution to yield strength will be considered here; a mean spacing proposed by Friedel (1964) (weak obstacles):

\[
\sigma_s = C_F \frac{a_s^{3/2}}{a_0} f^{1/2},
\]

(43)
a mean spacing according to the Mott–Labusch model, see Labusch (1970) and Neuhäuser and Schwink (2006) (strong obstacles):

\[ \sigma_s = C_L \frac{a_i^{4/3}}{a_0} f^{2/3}, \]  

(44)

and finally, the mean spacing given by Kocks for strong obstacles (see Deschamps and Brechet (1998) and references therein):

\[ \sigma_s = C_K \frac{a_i}{a_0} f^{1/2}. \]  

(45)

In Eqs. (43)–(45), \( a_0 \) denotes the expected mean particle size of all the \( N_p \) particles, and \( a_s \) refers to a representative size of the sheared particles in population \( N_s \). These quantities are evaluated as

\[ a_0 = \frac{1}{N_p} \sum_{i=1}^{N_p} a_i = \int_0^\infty a \cdot \text{pdf}(a) da, \quad a_s = \frac{1}{N_s} \sum_{i=1}^{N_s} a_i = \int_0^a_s a \cdot \text{pdf}(a) da, \]  

(46)

where pdf\( (a) \) denotes a probability density function of particle size.

The contribution from sheared particles to the overall yield strength will be added to the matrix material in an ad hoc manner. Eq. (30) modified to include sheared particles is then taken as

\[ \sigma_c \leq \frac{(1 - f_s)}{(1 - f_s)} \left[ \sigma_m(\varepsilon^p_c) + \sigma_e \right] + \frac{3f_s \sigma_0 \widetilde{\alpha} \varepsilon}{(1 - f_s) a_s^2} + \frac{3 \tilde{G}_f b}{(1 - f_s) a_s^2}. \]  

(47)

Recall that \( \varepsilon_c^p = \varepsilon_c^p/(1 - f) \), and note that \( f_s \) replaces \( f \) in Eq. (30) and that the effective properties are evaluated in the same manner as described in Section 3 by replacing \( N_p \) with \( N_s \). Eq. (47) serves as an extension of Eq. (30) where the strengthening effect of shearable particles is accounted for. Formally the model has five parameters: \( \tilde{a} \varepsilon, a_s, C, \varepsilon, \varepsilon_T \) that need to be calibrated from experimental results. However, \( C \) should not be viewed as a free parameter. For a material with a monodispersion of particles with volume fraction \( f \), the contribution from shearable particles \( \sigma_c \) should, at the onset of macroscopic yield, be equal to the contribution from impenetrable particles when their size equals the critical radius \( a_c \). This reflects the notion that the obstacle strength from shearable and non-shearable particles are assumed to be the same at the critical radius \( a_c \), cf. Deschamps and Brechet (1998). In the current model, this implies that

\[ \sigma_c = \frac{3f_s \sigma_0 \varepsilon}{(1 - f) a_s^2}, \]  

(48)

where \( C \) enters the left-hand side of Eq. (48) in a manner dependent on the choice of \( \sigma_c \) from Eqs. (43)–(45). In practice, materials typically contain particles exhibiting a size distribution, for such cases \( f \) in Eq. (48) must be chosen judiciously.

6. Experimental validation of upper bound solution extended with shearing particles

To verify the proposed model, a comparison with uniaxial tensile data from Fazeli et al. (2008a) on an aged hardened \( Al - 2.8\text{wt\%Mg} - 0.16\text{wt\%Sc} \) alloy was performed. The tensile data corresponds to a peak hardened sample (PA) with a volume fraction \( f_{PA} \) = 0.45% of spherical \( Al_3Sc \) precipitates with average radius 1.8 nm, and an over aged sample (OA) with a precipitate volume fraction \( f_{OA} \) = 0.37% and average radius equal to 6.4 nm. Flow properties for the \( Al \) matrix material was taken from Jobba et al. (2015). The tensile tests performed in Fazeli et al. (2008a) and Jobba et al. (2015) were conducted at temperature 77 K. This choice of test temperature was selected to minimize additional growth of precipitates during straining (dynamic strain ageing), cf. Fazeli et al. (2008a). All input parameters used for the \( Al - 2.8\text{wt\%Mg} - 0.16\text{wt\%Sc} \) alloy are summarized in Table 1.

The precipitate size distributions with corresponding log-normal fits, as illustrated in Fig. 13, were created from the data in Fazeli et al. (2008b) using the Matlab functions1 histfit and fitdist. The log-normal probability density fits were then used instead of the raw data when calculating quantities dependent on precipitate size. Moreover, the yield stress contribution from shearable particles was included using Eq. (45), i.e. the model based on Kocks statistics.

Illustrated in Fig. 14 is the outcome of model comparison against experimental data. Formally, the model has four tunable parameters \( \tilde{a} \varepsilon, a_s, C, \varepsilon_T \). However, analyses of the influence of parameters have shown that the dependency on \( \varepsilon \) and \( \varepsilon_T \) is weak.

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Therefore, the choice of \( \omega = 1 \), cf. Eq. (19), has been used in the current fitting process. This corresponds to a reduction to two free parameters, \( \alpha \) and \( \bar{\alpha} \). The model was fitted to the experimental data using the Matlab function \texttt{lsqcurvefit}. Since the proposed model can only operate within a small strain regime, the fitting algorithm was carried out between 0.2% and 7.5% plastic strain. The resulting fitting parameters are summarized in Table 2. As seen in Fig. 14(a), the model can be fitted against the experimental data quite well. Due to the low volume fractions, the work hardening contribution from particles is not as easy to see compared to the effect on yield stress. However, as illustrated in Fig. 14(b), where the differences in yield stress have been eliminated, a significant contribution to work hardening is produced by the model in the case of an over aged sample, reflecting the increased storage of dislocations around non shearable particles. On the contrary, the model for the peak aged sample only shows a very small deviation from the base material in terms of work hardening, suggesting that most particles are shearable. The latter is corroborated by \( \bar{\alpha} \) being equal to 4.07 nm. As a comparison, the authors in Fazeli et al. (2008a) obtained a value of \( \bar{\alpha} \) equal to 3.7 nm. The initially high work hardening seen in Fig. 14(a) for the PA sample cannot be captured by the current model using a constant \( \bar{\alpha} \). However, since the physical implications of a diminishing interface strength as predicted by Eq. (19), is still rather unclear to the authors, a constant value, equivalent to putting \( \bar{c} = 0 \), has been adopted. Moreover, the obtained value of \( \bar{\alpha} = 0.33 \mu \text{m} \) is in line with what was found in Asgharzadeh and Faleskog (2021a) for a similar material system using the forerunner of the model presented here.

### Table 2

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \alpha )</td>
<td>4.07 nm</td>
<td>Shearing/bypassing transition radius</td>
</tr>
<tr>
<td>( \bar{\alpha} )</td>
<td>0.33 ( \mu \text{m} )</td>
<td>Effective length scale</td>
</tr>
</tbody>
</table>

7. Summary and concluding remarks

The analytical model in Faleskog and Gudmundson (2021) for initial yield stress of materials reinforced by small elastic particles has been extended to predict strain hardening. The main result is presented in Eq. (30), which gives an analytical prediction for the stress–strain relationship at proportional loading. The closed form solution has large advantages in comparison to alternative computational methods. Parameter dependencies like volume fraction of particles, particle size and stiffness are easily estimated from Eq. (30). In the absence of interfacial softening, the model predicts a linear hardening contribution from non shearable particles. This result is in line with the classic continuum models in Tanaka and Mori (1970) and Brown and Stobbs (1971). Numerical validation of the model was conducted using a 2D axisymmetric- and a 3D-cubic FEM model. In the 3D model, the particles were allowed to vary in both size and elastic properties. As a final validation, the UBS-model was tested against experimental data. The numerical simulations show that the UBS-model gives a highly accurate approximation to corresponding FEM solutions within a reasonably wide parameter space (see error maps in Figs. 8–9). The reason for the breakdown of the UBS-model is twofold. Firstly, as the volume fraction increases, the particles can no longer be regarded as isolated and the Eshelby formalism loses its validity. Secondly, at a certain level of stress, the plastic strain field becomes increasingly non uniform and significant gradients throughout the matrix follows. Since this violates the underlying assumption of a uniform plastic strain, a significant deviation from the FEM solutions follows. This effect appears however at quite large plastic strains, typically an order of magnitude larger (or more) than the composite yield strain \( \varepsilon_{\gamma 0} \). For lower strains, the upper bound solution shows excellent agreement with corresponding FEM solutions.
An approximate expression for the strain at which the plastic strain field starts to show significant non-uniformity has been given by Eq. (42) for materials with a perfectly plastic matrix. Noteworthy is that as the plastic strain becomes increasingly non-uniform, the macroscopic stress transitions from linear hardening until it reaches a constant saturation stress. This behaviour is very similar to what has been consistently observed in tensile tests of alloys containing hard second phase particles and can physically be tied to the process of plastic relaxation. In the current work, a purely phenomenological approach is adopted to account for stress saturation by introducing a transition function defined by Eq. (41). To account for shearable particles, the UBS-model was augmented in an ad hoc manner by adding the shearable yield stress contribution to the matrix flow stress.

The UBS-model was finally fitted to experimental data on an Al–2.8wt%Mg–0.16wt%Sc alloy heat treated to produce a peak aged sample containing a precipitate volume fraction of \( f = 0.45\% \) spherical precipitates with mean radius \( \bar{r} = 1.8 \text{ nm} \) and an over aged sample with corresponding values \( f = 0.37\% \) and \( \bar{r} = 6.4 \text{ nm} \). Kocks statistics was used to account for shearable precipitates. Very good agreement between model and experimental data was achieved with resulting fitting parameters in line with results from previous research. A more rigorous test of the UBS-model against experimental data, using samples subjected to several different ageing times and containing much larger precipitate volume fractions, will be published in a forthcoming paper.

CRediT authorship contribution statement

Philip Croné: Conceptualization, Methodology, Software, Validation, Formal analysis, Writing – original draft. Peter Gudmundsson: Conceptualization, Methodology, Validation, Formal analysis, Writing – original draft. Jonas Faleskog: Conceptualization, Methodology, Software, Validation, Formal analysis, Writing – original draft.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix. Stress in an ellipsoidal inclusion

A linear elastic ellipsoidal inhomogeneity (a particle with different elastic properties than the matrix) in an infinite solid (matrix) is considered. A uniform stress \( \sigma_{ij}^\infty \) is applied at infinity that corresponds to a uniform strain \( \varepsilon_{ij}^\infty \). In addition, a homogeneous plastic strain field \( \varepsilon_{ij}^p \) exists in the matrix. The plastic strain field will give rise to an eigenstrain \( \bar{\varepsilon}_{ij} = -\varepsilon_{ij}^p \) in the inhomogeneity. This relation can be understood from Fig. A.1, which illustrates the distribution of total strains in the solid resulting from a homogeneous plastic strain field in the matrix. The problem may be split up into two sub-problems where the total strains in the real problem are...
For a spherical inclusion, with an Eshelby tensor given on matrix form as (cf. Mura (1987))

\[ \varepsilon_m = C_m\varepsilon^e_m, \quad \varepsilon_p = C_p\varepsilon^e_p \]

\[ \sigma_m = C_m\varepsilon^c_m, \quad \sigma_p = C_p\varepsilon^c_p \]

(I): \( \sigma \neq 0 \)

(II): \( \sigma = 0 \)

\[ \sigma = C_p(\varepsilon^\infty + \varepsilon - \tilde{\varepsilon}) \]

\[ \text{where } \sigma = [\sigma_1, \sigma_2, \sigma_3]^T \text{ is the principal stress vector in the particle, } \varepsilon^\infty = [\varepsilon_1^\infty, \varepsilon_2^\infty, \varepsilon_3^\infty]^T, \quad \varepsilon = [\varepsilon_1, \varepsilon_2, \varepsilon_3]^T \text{ denotes the strain disturbance due to the presence of an inhomogeneity (particle), } \tilde{\varepsilon} = [\tilde{\varepsilon}_1, \tilde{\varepsilon}_2, \tilde{\varepsilon}_3]^T \text{ denotes the eigenstrain due to plastic straining in the matrix material, and } C_p \text{ is the elastic stiffness matrix of the particle defined by elastic modulus } E_p \text{ and Poisson’s ratio } \nu_p \text{ (} G_p = E_p / [2(1+\nu_p)] \text{).} \]

The stress in the inhomogeneity can be simulated by an equivalent inclusion problem where the whole solid is homogeneous with elastic modulus \( C_m \) everywhere, and by adding an equivalent (fictitious) eigenstrain \( \varepsilon^* \) to the known eigenstrain \( \tilde{\varepsilon} \). Hence,

\[ \sigma = C_m(\varepsilon^\infty + \varepsilon - \tilde{\varepsilon} - \varepsilon^*) \]

The stiffness matrix \( C_m \) is defined by elastic modulus \( E_m \) and Poisson’s ratio \( \nu_m \) (\( G_m = E_m / [2(1+\nu_m)] \)), and represents the properties of the matrix material. Since, \( \tilde{\varepsilon} \) is uniform in the particle and \( \varepsilon^\infty \) is uniform in the solid, the sum of the eigenstrains is also uniform in the particle and related to the strain disturbance as

\[ \varepsilon = S(\tilde{\varepsilon} + \varepsilon^*). \]

Here, \( S \) is the Eshelby tensor given on \( 3 \times 3 \) matrix form. Equivalency of stresses and strains in the two problems requires that

\[ C_p(\varepsilon^\infty + \varepsilon - \tilde{\varepsilon}) = C_m(\varepsilon^\infty + \varepsilon - \tilde{\varepsilon} - \varepsilon^*). \]

Substitution of \( (A.51) \) into \( (A.52) \) and solving for the equivalent eigenstrain gives after some manipulation

\[ \varepsilon^* = (Q - S)^{-1}\varepsilon^\infty + (Q - S)^{-1} (S-I) \tilde{\varepsilon}. \]

where \( Q = (C_m - C_p)^{-1}C_m \) has been introduced, and \( I \) is a \( 3 \times 3 \) identity matrix. Insertion of \( (A.53) \) into \( (A.51) \) then gives the strain disturbance

\[ \varepsilon = S(Q - S)^{-1}\varepsilon^\infty + (S+S(Q-S)^{-1} (S-I)) \tilde{\varepsilon}. \]

By the replacements \( \varepsilon^\infty = C_m^{-1}\sigma^\infty \) and \( \tilde{\varepsilon} = -\varepsilon^p \), the total stress in the particle can now be calculated by substitution of Eqs. \( (A.53) \) and \( (A.54) \) into Eq. \( (A.49) \), which gives

\[ \sigma = C_pQ(Q-S)^{-1}C_m^{-1}\sigma^\infty + C_pQ(Q-S)^{-1}(S-I)\varepsilon^p. \]

For a spherical inclusion, with an Eshelby tensor given on matrix form as (cf. Mura (1987))

\[ S = \begin{bmatrix} s_1 & s_2 & s_2 \\ s_2 & s_1 & s_2 \\ s_2 & s_2 & s_1 \end{bmatrix}, \quad s_1 = \frac{7-5\nu_m}{15(1-\nu_m)}, \quad s_2 = \frac{5\nu_m-1}{15(1-\nu_m)}. \]
matrices $\Phi_\infty$ and $\Phi_p$ take the simple forms

$$
\Phi_\infty = \begin{bmatrix}
1 & 1 & g_2 \\
1 & 1 & g_1 \\
g_2 & g_1 & g_1
\end{bmatrix}, \quad \Phi_p = \begin{bmatrix}
p_1 & p_2 & p_2 \\
p_2 & p_1 & p_2 \\
p_2 & p_2 & p_1
\end{bmatrix}.
$$

(A.57)

It is desirable to split the resulting stress in the particle into a hydrostatic part and a deviatoric part. This can be done by means of the matrices,

$$
H = \frac{1}{3} \begin{bmatrix}
1 & 1 & 1 \\
1 & 1 & 1 \\
1 & 1 & 1
\end{bmatrix}, \quad D = \frac{1}{3} \begin{bmatrix}
2 & -1 & -1 \\
-1 & 2 & -1 \\
-1 & -1 & 2
\end{bmatrix},
$$

(A.58)

which have the properties $I = H + D$, $HD = DH = 0$, $HH = H$, and $DD = D$. Recognizing that the mean (hydrostatic) value and the deviatoric part of a vector $v$, $v_h$ and $v'$, respectively, are brought out by the operations $Hv = v_h i$, with $i = [1, 1, 1]^T$, and $Dv = v'$, the total stress in the particle can be recast as

$$
\sigma = (H + D) \Phi_\infty (H + D) \sigma_\infty + (H + D) \Phi_p (H + D) \epsilon^p = \left( A \sigma_h + 3K \epsilon^p \right) i + \Gamma \sigma_\infty + 2Ge^p i',
$$

(A.59)

where

$$
A = g_1 + 2g_2 = \frac{3g(1 - v_m)}{2(1 - 2\nu_p) + g(1 - v_m)},
$$

$$
I = g_1 - g_2 = \frac{15g(1 - v_m)^2}{7 - 5v_m + 2(4 - 5v_m)g},
$$

$$
3K = p_1 + 2p_2 = \frac{1 - 2\nu_p + g(1 + v_m)/2}{E_p},
$$

$$
2G = p_1 - p_2 = \frac{2(1 + v_m) + 4g(4 - 5v_m)(1 + v_m)}{7 - 5v_m + 2(4 - 5v_m)g},
$$

$$
\epsilon^p = E_p / E_m, \quad g = G_p / G_m.
$$

Note that, $\epsilon_h^p = 0$ in (A.59), since $\epsilon^p$ is deviatoric.

References


