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Microscopic plasticity and damage in multi-phase steels: on the competing role of crystallography and phase contrast

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Abstract

This paper unravels micromechanical aspects of multi-phase metals whose microstructure comprises grains of two or more phases. The local plastic response is determined by (i) the relative misorientation of the slip systems of individual grains, and (ii) the different mechanical properties of the phases. The relative importance of these two mechanisms is unclear: is the plastic response dominated by the grain’s anisotropy, or is this effect overwhelmed by the mechanical incompatibility between the two phases? The answer impacts the modeling of such a material, but also gives insights in the resulting fracture mechanisms. Until now, this question has been addressed only for particular crystallographies and mechanical properties. In contrast, this paper presents a systematic study including a large set of distributions, crystallographies, and material parameters. It is found that the global and the plastic local response of the two extreme modeling choices (full crystal plasticity on one end and full isotropic plasticity on the other end) converge with increasing phase contrast. The effect of the crystallography is completely overwhelmed by the mechanical incompatibility when the yield stress of the hard phase is a factor of four higher compared to the soft phase. When this ratio is lower than two, its influence may not be neglected. However, even in this regime, fracture initiation is controlled by the local arrangement of phases. The latter is quantified in this paper through the average arrangement of phases around fracture initiation sites.

Keywords: crystal plasticity; multi-phase materials; micromechanics; ductile damage

1 Introduction

This paper studies the plastic response of multi-phase metals that macroscopically combine good strength and ductility. The microstructure typically comprises several phases that can be roughly classified in a soft phase and a hard phase, which have a significantly different yield stress. We study the competition between plasticity due to the misalignment of the slip systems of the grains, and that due to the contrast in mechanical properties between the two phases. We aim to determine their relative influence on the plastic response and the ductile damage of the matrix, at the level of an aggregate of grains, whereby we investigate of a – much simpler and less expensive – isotropic plasticity model provides sufficiently accurate predictions. Earlier works in this direction mainly focused on a single set of parameters or microstructures. In contrast, we consider a statistically relevant set of random microstructures for a wide range of parameters, thereby conciliating apparently contradictory conclusions in different regimes. The outcome of this analysis offers perspective to the required level of constitutive detail at this level of observation, for which a wide variety of models have been applied by different authors.

Materials that belong to the category of interest are metal-matrix composites and advanced high strength steels. The former has an aluminum matrix reinforced by silicon-carbide. It was recognized that the response is dominated mostly by the strong contrast in properties of the two constituents. The crystallography of the matrix was found to matter only at the final stages of deformation where fracture initiates [1–3]. Advanced high strength steels have a considerably more complicated, fully metallic, microstructure, whereby the main
mechanical contributions originate from the (soft) ferrite and the (hard) martensite phase. These steels display many phenomena which cannot be trivially explained by the theory and models that have been proposed for the, more simple, metal-matrix composites. Existing models were extended with more realistic microstructures [e.g. 4–6] but also with more realistic constitutive models, often involving crystal plasticity [e.g. 7–9].

For single phase materials, the effects of crystallography are significant on the plastic and damage response, as the misalignment of grains introduces mechanical contrast [10]. The natural question that arises is to what extent the phase contrast in multi-phase materials dominates this ‘misalignment contrast’. It is known that for the case of rigid particles embedded in an elasto-plastic matrix the micromechanical response is mostly controlled by the interaction of the particles and the matrix phase, whereas the crystallography is less important [1, 2, 11]. Experimentally, this has been considered only using a rigid fiber in an analog matrix material (silver chloride) [11], whereby transmission electron microscopy measurements were compared to isotropic elasto-plastic simulations. A satisfactory accuracy of the model predictions compared to the experiments was found except on the sub-grain level. If also the hard phase deforms plastically, the crystallography appears to play an important role that may not be neglected [7, 12].

These studies were based on a specific set of crystallographies, with parameters (mechanical and crystallographic / morphological) reflecting extreme cases. This paper considers a much wider range of parameters to identify where the two extreme regimes break down. The analysis is extended to the initiation of fracture for which the outcome of the competition between crystallography and phase contrast is yet undetermined. For this case in particular it is imperative to consider a large set of microstructures.

This paper is structured as follows. The microstructural model and the crystal and isotropic plasticity models are introduced in Sections 2 and 3. The macroscopic and microscopic elasto-plastic responses for these two models are compared in Section 4 for a wide range of hard phase volume fractions and phase contrasts. This comparison is extended to the initiation of ductile fracture in Section 5. The paper ends with concluding remarks in Section 6.

Nomenclature

\[
\begin{align*}
\langle a \rangle & \quad \text{ensemble average} \\
\bar{a} & \quad \text{volume average} \\
A & \quad \text{second order tensor} \\
\Lambda & \quad \text{fourth order tensor} \\
C = A \otimes B & \quad \text{dyadic tensor product} \\
C = A : B & \quad \text{single tensor contraction} \\
c = A : B = A_{ij}B_{ji} & \quad \text{double tensor contraction}
\end{align*}
\]

2 Microstructural model

2.1 Microstructure and spatial discretization

The microstructure is represented by an idealized periodic unit cell consisting of $32 \times 32$ equi-sized “grains”, of which an example is shown in Figure 1(a). Each grain is randomly assigned the properties of the hard or the soft phase, by comparing a random number in the range $[0,1]$ to a target volume fraction of the hard phase, $\phi_{\text{hard}}$. The crystallography of the grains is discussed in the next section. To obtain statistically representative results, an ensemble of 256 of these random unit cells is considered for each set of parameters. A reference value $\phi_{\text{hard}} = 0.25$ is considered, resulting in an ensemble average volume fraction $\langle \phi_{\text{hard}} \rangle = 0.25 \pm 0.04$.

Consistent with the adopted idealization, only grain averaged (tensorial) quantities are considered. A finite element based solution scheme is used, whereby the spatial discretization is chosen such that these quantities are converged to within 1% error. Each grain is discretized using $2 \times 2$ eight node bi-quadratic quadrilateral elements (see Figure 1(b)), each of which is numerically integrated using four Gauss points.
Figure 1. (a) A typical microstructure from the ensemble with a hard phase volume fraction $\phi^\text{hard} = 0.25$, whereby the grains of the two phases are shown in blue and red. (b) The numerical discretization within a single grain.

2.2 Macroscopic deformation and periodicity

The periodicity of the unit cell is applied using standard periodic boundary conditions. The displacement fluctuations are constrained such that the average deformation gradient tensor equals the prescribed macroscopic deformation gradient $\bar{F}$. Plane strain is assumed for the out-of-plane direction.

To concentrate on the local effects in the microstructure, an isochoric macroscopic deformation is applied. This way, any local volumetric deformation – resulting in a non-zero hydrostatic stress – can be directly linked to the local microstructural features. Pure shear is used for this purpose, which corresponds to the following logarithmic strain tensor

$$\bar{\varepsilon} = \sqrt{3} \frac{1}{2} \bar{\varepsilon} (\bar{e}_x \bar{e}_x - \bar{e}_y \bar{e}_y)$$

(1)

where $\bar{\varepsilon}$ represents the equivalent logarithmic strain. To introduce sufficient plastic deformation, $\bar{\varepsilon} = 0.2$ is used (applied in 2000 steps for an accurate time integration, see below).

3 Constitutive models

3.1 Introduction

The response of a standard crystal plasticity model is compared to an isotropic plasticity model. For both models, a rate-dependent formulation is adopted. This choice is classical for crystal plasticity, since it regularizes the slip system activation, while the choice for the isotropic plasticity model is made here for consistency. The parameters are chosen such that the resulting response is close to the rate-independent limit and such that both models coincide in the isotropic limit (i.e. an aggregate of grains with identical material properties). The actual values of the yield stress and hardening are therefore different for both constitutive models, even though the same symbols are used below.

Both models are formulated in a finite deformation setting, by assuming the multiplicative split of the deformation gradient, $F$, into an elastic part, $F_e$, and plastic part, $F_p$:

$$F = F_e \cdot F_p$$

(2)

This split introduces an intermediate configuration distorted by the plastic deformation only. The elastic deformation, as well as rotations, are included in $F_e$.

The plastic part of the velocity gradient is introduced as $L_p := \dot{F}_p \cdot F_p^{-1}$. Different expressions for $L_p$ are chosen for the crystal and the isotropic plasticity model, see below.

It is furthermore useful to introduce the pull-back of the Kirchhoff stress tensor $\tau$ to the intermediate configuration:

$$S_i = F_e^{-1} \cdot \tau \cdot F_e^{-T}$$

(3)
The elastic constitutive relation for $S_i$ reads:

$$S_i = C : E_e$$

for both crystal and isotropic plasticity. Herein, $C$ is the usual (isotropic) fourth-order elasticity tensor characterized by Young’s modulus $E$ and Poisson’s ratio $\nu$. $E_e := \frac{1}{2}(C_e - I)$ is the elastic Green-Lagrange strain, where $C_e := F_e^T \cdot F_e$ is the elastic Cauchy-Green tensor.

### 3.2 Crystal plasticity

Within a standard crystal plasticity formulation [13], the plastic part of the velocity gradient, $L_p$, is the sum of the plastic slip rates, $\dot{\gamma}_\alpha$, along the individual slip planes, $\alpha$:

$$L_p = \sum_{\alpha=1}^{n_s} \dot{\gamma}_\alpha P^\alpha_0$$

where $n_s$ is the number of slip systems; the Schmid tensor $P^\alpha_0$ defines the slip system’s orientation through $P^\alpha_0 := s^\alpha_0 \otimes n^\alpha_0$ where $s^\alpha_0$ is the slip direction and $n^\alpha_0$ is the normal to the slip plane in the intermediate configuration. For both the soft and the hard phase, the number of active slip systems $n_s = 12$, all belonging to the $\{110\}$ slip system family for body centered cubic crystals [see 14]. Non-Schmid effects are not considered. Throughout this paper, the grain orientations – i.e. the Euler angles – are selected randomly, such that the aggregate of grains is isotropic [e.g. 15].

The plastic slip rate along each slip system, $\dot{\gamma}_\alpha$, is determined via a visco-plastic slip law [16]

$$\dot{\gamma}_\alpha = \dot{\gamma}_0 \left( \frac{|\tau_\alpha|}{s_\alpha} \right)^{1/m} \text{sign}(\tau_\alpha)$$

where $\dot{\gamma}_0$ is a reference slip rate, $m$ is the strain rate sensitivity, and $\tau_\alpha$ is the resolved shear stress along the $\alpha$th slip system:

$$\tau_\alpha = (S_i \cdot C_e) : P^\alpha_0$$

The current slip resistance $s_\alpha$ is calculated via the following evolution law

$$\dot{s}_\alpha = \sum_{\beta=1}^{n_s} h_{\alpha\beta} |\dot{\gamma}_\beta|$$

which has an initial value of $s_0$. The hardening is a combination of self-hardening and latent hardening defined through the hardening matrix

$$h_{\alpha\beta} = h_0 \left( 1 - \frac{s_\alpha}{s_\infty} \right)^a \left( \delta_{\alpha\beta} + q_n (1 - \delta_{\alpha\beta}) \right)$$

where $q_n$ is the latent hardening over self-hardening ratio for non-coplanar slip systems and $\delta_{\alpha\beta}$ is the Kronecker delta; $h_0$, $s_\infty$ and $a$ are material parameters.

An equivalent plastic strain, $\varepsilon_p$, is defined for comparison purposes. Its evolution reads

$$\dot{\varepsilon}_p = \sqrt{\frac{2}{3} D_p : D_p}$$

Its initial value is naturally zero. This definition is similar to that of [7], where $L_p$ is instead.

### 3.3 Isotropic plasticity

For the case of isotropic plasticity, it is assumed that $L_p \equiv D_p$. The following expression of $D_p$ is employed [e.g. 17, 18]:

$$D_p = \frac{3}{2} \frac{\dot{\varepsilon}_p}{s_{eq}} S_i^d : C_e$$
Table 1. Used materials parameters for the crystal plasticity and the isotropic plasticity model.

| Model             | \( s_0 / E \) | \( s_\infty / E \) | \( h_0 / E \) | \( \dot{\gamma}_0 \) | \( a \) | \( m \) | \( q_n \) | \( \nu \) |
|-------------------|----------------|---------------------|----------------|-------------------|------|-----|-------|-----|
| Isotropic plasticity | 170            | 8000                | 70             | 0.01              | 1.5  | 0.1 | 1.4   | 0.3 |
| Crystal plasticity  | 450            | 8000                | 800            | 0.01              | 1.5  | 0.1 | -     | 0.3 |

where \( \dot{\varepsilon}_p \) is the equivalent plastic strain rate, and the equivalent stress \( s_{eq} \) is defined as follows

\[
s_{eq} = \sqrt{\frac{3}{2}(S^d \cdot C_e) : (S^d \cdot C_e)}
\]

where the stress deviator \( S^d = S_i - \frac{1}{3} (S_i : C_e) C_e^{-1} \) [cf. 18, 19]. The evolution of the plastic strain reads

\[
\dot{\varepsilon}_p = \dot{\gamma}_0 \left( \frac{s_{eq}}{s_y} \right)^{1/m}
\]

where the yield stress is given by

\[
s_y = s_0 + h \varepsilon_p
\]

and finally the hardening

\[
h = h_0 \left( 1 - \frac{s_y}{s_\infty} \right)^a
\]

3.4 Material parameters and phase contrast

The focus in this paper is on the plastic response, and hence the same (isotropic) elastic behavior is assumed for both models. To render the plastic response comparable, the parameters of the isotropic model are chosen representative for the considered class of materials [e.g. 20]. The soft phase is taken as a reference and the parameters of the hard phase are obtained by scaling them relative to the soft phase (see below). The constitutive response of the soft phase is plotted in Figure 2 using a solid red line, in terms of the equivalent Kirchhoff stress \( \bar{\tau}_{eq} \), as a function of the equivalent logarithmic strain \( \bar{\varepsilon} \). Next, the parameters of the crystal plasticity model are fitted such that the response coincides with that of the isotropic model in an average sense (for a unit cell of many randomly oriented grains of the soft phase). The resulting average response is plotted in Figure 2 using a solid green line. Note that crystal plasticity predicts a more gradual transition from the elastic to the plastic regime, as the slip planes of the different grains become active at various stages of deformation. After yielding, the predicted response of the two models is comparable. All parameters are listed in Table 1.

Most parameters of the hard phase are the same as those of the soft phase, except for the yield stresses and hardening moduli - \( s_0, s_\infty, \) and \( h_0 \) - which are scaled by a factor \( \chi = \frac{3}{2}, 2, 4, \) and \( 8 \). As an example, the behavior for \( \chi = 2 \) is shown in Figure 2 using dashed lines for both models. Note again that the plastic responses of both models closely resemble each other, except during initial yielding. A reference stress \( \tau_0 \), which coincides with the reference initial yield stress, is also introduced in Figure 2.

4 Elasto-plastic response

4.1 Macroscopic response

The model in which both phases are modeled using crystal plasticity and for which the hard phase volume fraction equals 0.25 is taken as the reference case. For this model, the scatter in the macroscopic response of the different unit cells in the ensemble is shown in Figure 3, whereby the lower- and upper-bound are highlighted. In this figure, the macroscopic equivalent Kirchhoff stress, \( \bar{\tau}_{eq} \), normalized by the reference stress, \( \tau_0 \), is plotted as a function of the applied average strain, \( \bar{\varepsilon} \), using different colors for different values
of phase contrast, \( \chi \). The yield stress is approximately constant while the hardening strongly increases with increasing \( \chi \). Also the scatter between different microstructures increases with \( \chi \). This behavior results from the sequence of plastic events activating in the microstructure. First, the soft phase starts yielding, while the hard phase remains elastic. Macroscopically this is observed as the onset of yielding. As a consequence of the hardening of the soft phase, the hard phase also starts to yield resulting in a higher macroscopic hardening than due to the soft phase only. Since the yield stress (including hardening) of the hard phase increases by increasing \( \chi \), more stress is required for the hard phase to yield, explaining the increased macroscopic hardening. Whether the hard phase yields is determined by local compatibility within the microstructure. Since the hard phase yields at a higher stress, the microstructural configuration becomes more important, which induces the observed increased scatter between the different microstructures.

The effect of using an isotropic model is shown in Figure 4 for an applied strain of \( \bar{\varepsilon} = 0.2 \). In Figure 4(a) the microstructural model is simplified by applying the isotropic model for either one or both phases for a
phase contrast $\chi = 3/2$. The scatter between the different microstructures is shown using a box-plot. (i) The reference crystal plasticity model is shown in black. From left to right: (ii) the soft phase is assumed isotropic while the hard phase remains plastically anisotropic; (iii) the hard phase is assumed isotropic while the soft phase remains plastically anisotropic, and finally, (iv) both phases are assumed isotropic. In the extreme case with both phases isotropic, the macroscopic response is harder with respect to the reference case where both phases are plastically anisotropic. Assuming the soft phase isotropic has a much bigger effect than assuming the hard phase isotropic (3% instead of 1% increase of $\bar{\tau}_{eq}$). This is logical, as the soft phase takes most of the plastic deformation.

Figure 4(b) shows the reference, crystal plasticity, model together with the strongest assumption where both phases are isotropic, as a function of phase contrast, $\chi$. For both cases the scatter between the different microstructures increases with $\chi$ (as was observed for Figure 3). A more important observation is that both models approach the same values. In terms of the ensemble average, the isotropic model predicts a 4% higher stress for $\chi = 3/2$ while this is reduced to 2% for $\chi = 8$. In terms of the scatter however, for $\chi = 3/2$ all unit cells predict a higher stress while for $\chi = 8$ only 7% of the unit cells predict a higher stress. This implies that if the contrast between the phases is large enough, assuming both phases isotropic is less relevant than the phase contrast in terms of mechanical properties. In term of the statistics of Figure 4(b) it is found that if $\chi \geq 4$ the stress predicted by the isotropic model is accurate for 80% of the unit cells.

4.2 Microscopic response

The local plastic response is shown in Figure 5 for a typical microstructure; all snapshots are taken at the same applied strain $\bar{\varepsilon} = 0.2$. The phase contrast, $\chi$, increases from left to right. For the two extremes, $\chi = 3/2$ and $\chi = 8$, a magnified region is shown in Figure 6. The reference model, where both phases are modeled with crystal plasticity, is shown in the top row, and the simplest approximation where both phases are isotropic is shown in the bottom row. In all cases, the plastic strain, $\varepsilon_p$, is higher in the soft phase than in the hard phase. This partitioning is most pronounced for the highest phase contrast ($\chi = 8$, Figures 5(d,h)) where almost no plastic strain is observed in the hard phase. The highest values of $\varepsilon_p$ are found within bands in the soft phase oriented under $\pm 45$ degrees, coinciding with the shear directions; this deformation localization increases with $\chi$.

In comparing the two models (crystal vs. isotropic plasticity) only minor differences are observed for the highest phase contrast $\chi = 8$ (cf. Figures 5,6(d,h)) both in the plastic strain, $\varepsilon_p$, and the (periodic)
displacements. Clear differences appear for lower $\chi$. In particular at the lowest phase contrast ($\chi = 3/2$), the displacements and the local plasticity are noticeably more homogeneous for the isotropic model (cf. Figures 5,6(a,e)). For the crystal plasticity model, fluctuations of $\varepsilon_p$ are observed from grain to grain within the soft phase, indicating that one grain is more favorably oriented than the other. The local orientation differences introduce an incompatibility which competes with the incompatibility due to the phase contrast.

Figure 5. The local equivalent plastic strain, $\varepsilon_p$, for increasing phase contrast $\chi$ (left to right) and different constitutive models: both phases modeled with crystal plasticity (top) and both with isotropic plasticity (bottom); all at an applied strain of $\bar{\varepsilon} = 0.2$ and the same microstructure (include crystallography) of Figure 1. Grains of the hard phase are highlighted using a black outline.

Figure 6. Zoom of Figure 5: (a,e) for $\chi = 3/2$ and (d,h) for $\chi = 8$.

To address the above observations systematically, the local responses of the entire ensemble is considered. In Figure 7 the probability density $\Phi$ of the plastic strain $\varepsilon_p$ (top) and hydrostatic stress $\tau_m$ (bottom) are shown for increasing phase contrast $\chi$ (left to right). The plots include $\Phi$ of the ensemble of grains (thick solid line), as well as that of only the hard phase (thin solid line) and of only the soft phase (thin dashed line) – for the reference crystal plasticity model (black) and the isotropic model (blue).
For the plastic strain (top) it is observed that the partitioning between the hard and the soft phase increases with increasing $\chi$: the soft phase accumulates more deformation. At the same time the scatter increases, implying that the plasticity is more localized. When the isotropic approximation (blue) is compared to the reference model (black), it is observed that the two tend to overlap with increasing $\chi$. This also holds for the plastic strain distribution within each phase.

For the hydrostatic stress (bottom), the amplitude is similar in the hard and the soft phase. Note that both phases have the same elastic response, justifying the comparable amplitudes. As the macroscopic deformation introduces no global hydrostatic stress, any non-zero hydrostatic stress is related to the inhomogeneity of the microstructure only. Similarly as for the hard phase, the hydrostatic stress in the isotropic approximation approaches that of the reference crystal plasticity model for increasing $\chi$.

Figure 7. The ensemble probability density $\Phi$ of the local plastic strain $\varepsilon_p$ (top) and the local hydrostatic stress $\tau_m$ (bottom) at an applied strain $\varepsilon = 0.2$. The phase contrast $\chi$ increases from left to right. The isolated hard phase (thin solid line) and soft phase (thin dashed line) are normalized with respect to their respective volume fractions. The different constitutive assumptions are plotted using a different color: black for crystal plasticity and blue for isotropic plasticity.

4.3 Influence of the hard phase volume fraction

The analysis is next extended to different ranges of hard phase volume fraction, i.e. $\varphi^{\text{hard}} = 0.50$ and 0.75. For the reference (crystal plasticity) model, the macroscopic response is shown in Figure 8(a) using different colors for the different hard phase volume fractions; all ensembles have the same phase contrast $\chi = 3/2$. The initial yield stress and the hardening increase with the hard phase volume fraction, as to be expected from the rule of mixtures. The response at an applied strain $\varepsilon = 0.2$ is shown for the full range of considered parameters in Figure 8(b), where the macroscopic stress, $\tau_{eq}$, is plotted as a function of the hard phase volume fraction, $\varphi^{\text{hard}}$, using a marker for each individual unit cell. The figure shows the strong combined influence of the hard phase volume fraction and phase contrast. The dependence on the volume fraction is clearly more pronounced for a larger phase contrast. For $\chi = 8$, $\tau_{eq}$ scales approximately with a factor $\chi \varphi^{\text{hard}}$. For $\chi = 3/2$, it only scales with 50% thereof. An empirical power-law scaling relation of the macroscopic stress relative to the volume fraction (with an exponent of approximately 1.3) can thus be extracted from the responses.

The microstructural response is studied in a more coherent way by considering the distribution of the plastic strain and hydrostatic stress response of all grains in the ensembles, as a function of phase contrast
Figure 8. (a) The range of the normalized macroscopic equivalent stress, $\tau_{eq}$, as a function of the applied equivalent strain, $\bar{\varepsilon}$, of the individual unit cells, for different hard volume fractions, $\varphi_{\text{hard}}$, all for a phase contrast $\chi = 3/2$. (b) The response of the individual unit cells at $\bar{\varepsilon} = 0.2$ for all parameter variations. The two phases are modeled with crystal plasticity.

$\chi$. Figure 9 shows the distribution (confidence intervals) per phase: soft (blue) and hard (red). The solid lines correspond to the crystal plasticity model while the dashed lines correspond to the isotropic model. Figures 9(a–c) show the equivalent plastic strain, $\varepsilon_p$, and Figures 9(d–f) show the hydrostatic stress, $\tau_m$. From left to right the volume fraction increases. From the results it is observed that in each case the difference between the two models reduces with increasing phase contrast $\chi$. For $\varphi_{\text{hard}} = 0.25$, the range of plastic strain is a factor of 2.2 (soft phase) and 2.4 (hard phase) more narrow for the isotropic model than for the crystal plasticity model for the lowest phase contrast, $\chi = 3/2$. In the other extreme, $\chi = 8$, these ratios reduce to 1.1 and 1.3, respectively. This is consistently observed also for the hydrostatic stress where for $\chi = 3/2$ the ratio is 2.0 for the soft phase and 1.9 for the hard phase, while they are reduced to 1.1 and 1.05 for $\chi = 8$. This trend is confirmed for $\varphi_{\text{hard}} = 0.5$. For the highest hard phase volume fraction, $\varphi_{\text{hard}} = 0.75$, however the range of plastic strains in the soft phase appears to be overestimated by the isotropic model for $\chi = 8$ (see Figure 9(c)) with a factor 1.1 for the soft phase and 1.01 for the hard phase, whereas the range of hydrostatic stress is underestimated by the isotropic model in both phases (with a factor of 1.2 for the soft phase and 1.3 for the hard phase, see Figure 9(f)). The mismatch originates from the fact that at this high hard phase volume fraction the hard phase starts to form a network across the unit cell. In that case, the hard phase is forced to significantly deform plastically also at the highest $\chi$. The soft phase follows the hard phase, through the strong constraint acting on it.

4.4 Effect of planar assumption

So far, plane strain conditions have been assumed, thereby artificially constraining the crystals. To assess the consequences thereof, the microstructure is extended to a quasi-three-dimensional setting, whereby the finite element discretization is three-dimensional but the microstructure stays two-dimensional. In this case, periodicity is used in all three spatial directions, whereby the average deformation gradient tensor $\bar{\varepsilon}$ is given by equation (1). The deformation is thus constrained to be planar only on average, allowing for local out-of-plane deformations. The analysis is performed using a hard phase volume fraction $\varphi_{\text{hard}} = 0.25$.

For the reference, crystal plasticity, model the scatter of the 3-D macroscopic responses is shown in Figure 10, along with the two-dimensional results. As expected, the response is more compliant now that the system is less constrained. In the local response, depicted in Figure 11, the out-of-plane displacements are clearly visible. However, the equivalent plastic strain distribution remains comparable to the two-dimensional case (cf. Figures 11 and 5).

The local response of the ensembles with either a two- and three-dimensional discretization is systemati-
Figure 9. The distribution (average ± standard deviation) of the equivalent plastic strains $\varepsilon_p$ (top) and hydrostatic stresses $\tau_m$ (bottom) in the ensemble, as a function of the phase contrast $\chi$. From left to right the volume fraction increases. Colors are used to discriminate between the hard phase (red) and soft phase (blue). The line-style corresponds to the constitutive model: both phases modeled with crystal plasticity (solid) and both phases with isotropic plasticity (dashed). All figures are at $\bar{\varepsilon} = 0.2$.

Figure 10. Macroscopic equivalent stress $\tau_{eq}$ as a function of applied equivalent strain $\bar{\varepsilon}$ for the two-dimensional spatial discretization and the three-dimensional (fully periodic) spatial discretization. Both phases are modeled with crystal plasticity, a hard phase volume fraction $\varphi_{\text{hard}} = 0.25$ and a phase contrast $\chi = 3/2$. 
Figure 11. Local plastic strain $\varepsilon_p$ for different values of the phase contrast $\chi$. Both phases are modeled with crystal plasticity, all figures are at an applied strain $\bar{\varepsilon} = 0.2$.

cally compared in Figure 12, for the plastic strain (top) and hydrostatic stress (bottom). The differences are minor, independent of the phase contrast $\chi$. The relative local difference in the response of the individual grains is at most 8%, which is slightly higher than what is observed macroscopically (6%).

4.5 Discussion

The results of the present study are consistent with earlier results in the literature. Both Needleman and Tvergaard [1] and McHugh et al. [2] using rigid reinforcement particles observed minor differences for an isotropic plasticity compared with a crystal plasticity model. This was experimentally confirmed by Nugent et al. [11]. This case corresponds best to a phase contrast of $\chi = 8$ in the present study, for which the same observations are revealed. If the reinforcement phase is no longer rigid, Choi et al. [7] observed distinct differences between the isotropic and the reference crystal plasticity model. Their parameters compare with a phase contrast of $\chi = 3/2$ in the present study for which indeed clear differences appeared. Based on the results presented here, the apparently contradictory observations in the literature stem from the fact that each considers a clearly different regime for the phase contrast.

It may thus be concluded that if the mechanical contrast $\chi$ between the two phases is sufficiently high, the effect of the orientation discontinuity of the slip systems between individual grains is smaller or even negligible – both in the volumetric and the deviatoric response. If the phase contrast is low, the incompatibility between the phases competes with the incompatibility introduced by the orientation mismatch of the different crystals. Consequently, using isotropic plasticity is particularly meaningful for high phase contrasts. It can be used with an adequate quantitative approximation for $\chi \geq 4$. This conclusion also holds for different hard phase volume fractions, where the hard phase may no longer be considered as a reinforcement phase. Furthermore, relaxing the out-of-plane constraint has a negligible influence on these observations.

For the phase contrast $\chi = 3/2$, where the crystallography plays an important role, it remains questionable whether the anisotropy of both phases has equal influence on the mechanical response. To this end, the reference ensemble is compared with two approximations in which only one of the two phases is assumed isotropic. The result is shown in Figure 13 in terms of the ensemble probability density $\Phi$ of the equivalent plastic strain $\varepsilon_p$ (top) and the hydrostatic stress $\tau_m$ (bottom). When the hard phase is assumed isotropic (left), the plastic strain in the hard phase becomes more homogeneous; the plastic strain in the soft phase and the hydrostatic stress in both phases are not affected. On the other hand, if the soft phase is assumed isotropic only the plastic strain in the hard phase is unaffected. Both the plastic strain in the soft phase as well as the hydrostatic stress in both phases are significantly different. This observation is particularly interesting in the context of advanced high strength steels (the properties of which are in this range) as different researchers have confirmed that martensite, which acts as reinforcement phase, may be highly anisotropic in the plastic domain [21–23].
Figure 12. Effect of out-of-plane constraints on the local response. Both phases modeled with crystal plasticity, $\varphi_{\text{hard}} = 0.25$.

Figure 13. The probability density $\Phi$ of the plastic strain $\varepsilon_p$ and hydrostatic stress $\tau_m$ for the case where only one of the phases is isotropic: (a,c) the hard phase and (b,d) the soft phase. The phase contrast $\chi = 3/2$, the hard phase volume fraction $\varphi_{\text{hard}} = 0.25$, and the applied strain $\bar{\varepsilon} = 0.2$. 
5 Ductile damage

5.1 Introduction
The analysis is finally extended to ductile fracture whereby emphasis is placed on two-phase steels where the hard phase acts as a reinforcement of the softer ductile matrix. Consequently, the hard phase volume fraction is fixed to $\varphi^{\text{hard}} = 0.25$. The soft matrix is assumed to fail by ductile fracture while the hard phase is assumed not to fracture. Many different criteria exist for ductile fracture initiation, but they are all dependent on a non-linear combination of the plastic strain and hydrostatic stress [e.g. 24–26]. For this reason it may be expected that subtle inaccuracies of these quantities due to the constitutive choice (isotropic instead of crystal plasticity) may be more influential for ductile fracture initiation.

5.2 Damage indicator
The Johnson-Cook damage indicator [26] is used to indicate the onset of ductile fracture in the soft phase. This indicator, $D$, signals fracture initiation once $D \geq 1$, but does not weaken the material response. It is defined as follows:

$$ D = \int_0^T \frac{\dot{\varepsilon}_p}{\varepsilon_c(\eta)} \, d\tau $$

where $\dot{\varepsilon}_p$ is the equivalent plastic strain rate and $\varepsilon_c$ is a critical strain which depends on the local stress triaxiality $\eta$ in the following way

$$ \varepsilon_c = A \exp(-B\eta) + \varepsilon_{pc} $$

wherein $A$, $B$, and the critical plastic strain $\varepsilon_{pc}$ are material parameters. The stress triaxiality is the ratio of hydrostatic and equivalent (shear) Kirchhoff stress in the grain:

$$ \eta = \frac{\tau_m}{\tau_{eq}} $$

The parameters are chosen representative for the considered class of materials, based on the literature [20]:

$$ A = 0.2 \quad B = 1.7 \quad \varepsilon_{pc} = 0.1 $$

Note that the exact choice of parameters is not essential for the purpose of this study, however choosing them in a correct range leads to a more comprehensive interpretation of the value of $D$.

5.3 Microscopic response
For the microstructure presented earlier in Figures 1 and 5, the damage indicator $D$ is shown in Figure 14 for different values of the phase contrast $\chi$ (at the same applied strain $\bar{\varepsilon} = 0.2$). Due to the increasing phase contrast $\chi$, the damage indicator also increases, indicating that a higher phase contrast promotes damage. Furthermore, the damage is more localized for higher $\chi$. It is particularly high near the interfaces of the hard and the soft phase (discussed in more detail in [27]). In a large part of the shear bands that are observed in Figure 5, $D$ is significantly lower than one.

The importance of the plastic anisotropy is assessed by comparing the assumption of plastic isotropy to the reference crystal plasticity model. Figure 15 shows the probability density function $\Phi$ of the damage $D$ for different levels of phase contrast $\chi$. The reference model is shown in black, while the isotropic model is shown in blue. For the lowest phase contrast, $\chi = 3/2$, there is a significant difference between the damage predicted by the two models, whereby the damage is considerably higher in the crystal plasticity model in 12% of the grains. The value of $D$ predicted by the two models converges with increasing $\chi$ (it is wrongly predicted in only 1% of the grains for $\chi = 8$). Based on these results, it may be concluded that for $\chi \geq 4$ there is no pronounced difference between isotropic and crystal plasticity, while for $\chi \leq 2$ the difference is significant.
Figure 14. The local damage indicator $D$ in the soft phase for different phase contrasts $\chi$. The microstructure and applied deformation is the same as in Figure 1, both phases are modeled with crystal plasticity.

Figure 15. The probability density $\Phi$ as a function of the damage indicator $D$ in the soft phase, for different values of the phase contrast $\chi$. The applied strain $\bar{\varepsilon} = 0.2$.

5.4 Effect of the morphology: damage hot-spot

Since the damage is dominated by the presence of the two phases, the question arises how their spatial distribution contributes to this, and whether this contribution is different when also the crystallography significantly contributes to damage. To quantify this, the average phase arrangement is characterized as a function of the position relative to the fracture initiation sites. Following De Geus et al. [27], the probability of finding the hard phase is calculated as a function of the position relative to the fracture initiation site. As only two phases are considered, the probability of finding the soft phase is implicitly contained in this result. If at a certain relative position the probability of hard phase is higher than the hard phase volume fraction, $\varphi_{\text{hard}}$, having hard phase at this relative position thus promotes fracture initiation. Likewise, if the probability is lower than $\varphi_{\text{hard}}$, having soft phase at that relative position promotes fracture initiation.

This method is discussed based on a single unit cell. The extension to the ensemble average is trivial. A phase indicator $I$ is introduced that describes the phase distribution as follows:

$$I(i, j) = \begin{cases} 1 & \text{for } (i, j) \in \text{hard} \\ 0 & \text{for } (i, j) \in \text{soft} \end{cases}$$ (20)

where $(i, j)$ is the position, here coinciding with the matrix-index of each grain. Similarly, fracture initiation is indicated by $D(i, j)$ which is one if the damage indicator $D(i, j) \geq 1$ and zero elsewhere. To correlate the arrangement of phases to the fracture initiation, the average value of $I$ is calculated at a certain position $(\Delta i, \Delta j)$ relative to the fracture initiation sites, where $D = 1$, as follows:

$$I_D(\Delta i, \Delta j) = \frac{\sum_{ij} D(i, j) I(i + \Delta i, j + \Delta j)}{\sum_{ij} D(i, j)}$$ (21)

where $(i, j)$ loops over all grains, taking the cell’s periodicity into account. The resulting damage hot-spot $I_D$
thus characterizes the probability of finding the hard phase at different positions \((\Delta i, \Delta j)\) relative to fracture initiation. The ensemble average \(\langle I_D \rangle\) trivially follows by looping over all grains in the ensemble.

The result is shown in Figure 16 for different phase contrasts \(\chi\), whereby the response to the crystal plasticity model is shown on the top row and the response to the isotropic plasticity model on the bottom row. The colormap has been chosen to enhance the interpretation, whereby red indicates an elevated probability of the hard phase and blue that of the soft phase, the neutral color (white) coincides with the hard phase volume fraction \(\phi_{\text{hard}}\) indicating no preferential phase at that position relative to damage. The results show that fracture initiates where regions of the hard phase are aligned with the tensile axis and interrupted by regions of the soft phase aligned with the shear direction at \(\pm 45\) degree angles (see [27], and reference therein, for a detailed mechanical analysis). Qualitatively the arrangement of phases around fracture initiation sites appears to be independent of the phase contrast and of the plastic (an)isotropy. Even though the influence of crystallography on the value of the damage, \(D\), may not be neglected for a low phase contrast; the spatial locations where fracture initiates are not affected by it.

![Figure 16.](image)

\textbf{Figure 16.} The average phase indicator around fracture initiation, \(I_D\), for different phase contrasts \(\chi\), for a hard phase volume fraction \(\phi_{\text{hard}} = 0.25\) and applied strain \(\varepsilon = 0.2\). The rows correspond to different constitutive choices: both phases modeled with crystal plasticity (top) or isotropic plasticity (bottom). The colormap is chosen such that the neutral color (white) coincides with the hard phase volume fraction. The color may be interpreted as: hard phase (red) and soft phase (blue).

6 Conclusions

The role that the plastic anisotropy, as introduced by the crystallography, plays on the micromechanical response of a two-phase material is carefully studied by comparing the response predicted by a crystal plasticity to that predicted using an isotropic formulation. The following observations have been made.

- The plastic anisotropy is less important than the mechanical incompatibility when the ratio of the yield stresses between the phases is larger than four. Below a ratio of two the influence of the orientation mismatch of the grains is significant. This has been assessed through the plastic strain and the hydrostatic stress. This confirms observations in the literature where only one of the regimes was analyzed independently [1, 2, 7].
• These observations also hold for the initiation of ductile fracture of the comparatively soft phase.

• The spatial arrangement of the phases plays a crucial role for the initiation of ductile fracture in the soft matrix phases [e.g. 2, 28]. The analysis showed that this effect dominates over the role of crystallography, even in the regime where its quantitative influence on the mechanical response may not be neglected.

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References

References

[1] A. Needleman and V. Tvergaard. Comparison of Crystal Plasticity and Isotropic Hardening Predictions for Metal-Matrix Composites. J. Appl. Mech., 60(1):70–76, 1993. doi: 10.1115/1.290781.

[2] P. E. McHugh, R. J. Asaro, and C. F. Shi. Computational modeling of metal matrix composite materials - I. Isothermal deformation patterns in ideal microstructures. Acta Metall. Mater., 41(5):1461–1476, 1993. doi: 10.1016/0956-7151(93)90255-Q.

[3] R. Aghababaei and S. P. Joshi. Grain size-inclusion size interaction in metal matrix composites using mechanism-based gradient crystal plasticity. Int. J. Solids Struct., 48(18):2585–2594, 2011. doi: 10.1016/j.ijsolstr.2011.05.012.

[4] K. S. Choi, W. N. Liu, X. Sun, and M. A. Khaleel. Influence of Martensite Mechanical Properties on Failure Mode and Ductility of Dual-Phase Steels. Metall. Mater. Trans. A. 40(4):796–809, 2009. doi: 10.1007/s11661-009-9792-6.

[5] X. Sun, K. S. Choi, A. Soulami, W. N. Liu, and M. A. Khaleel. On key factors influencing ductile fractures of dual phase (DP) steels. Mater. Sci. Eng. A. 526(1-2):140–149, 2009. doi: 10.1016/j.msea.2009.08.010.

[6] H. Kumar, C. L. Briant, and W. A. Curtin. Using microstructure reconstruction to model mechanical behavior in complex microstructures. Mech. Mater., 38(8-10):818–832, 2006. doi: 10.1016/j.mechmat.2005.06.030.

[7] S. H. Choi, E. Y. Kim, W. Woo, S. H. Han, and J. H. Kwak. The effect of crystallographic orientation on the micromechanical deformation and failure behaviors of DP980 steel during uniaxial tension. Int. J. Plast., 45:85–102, 2013. doi: 10.1016/j.ijplas.2012.11.013.

[8] D. D. Tjahjanto, S. Turteltaub, A. S. J. Suiker, and S. van der Zwaag. Modelling of the effects of grain orientation on transformation-induced plasticity in multiphase carbon steels. Model. Simul. Mater. Sci. Eng., 14(4):617–636, 2006. doi: 10.1088/0965-0393/14/4/006.

[9] F. Roters, P. Eisenlohr, L. Hantherli, D. D. Tjahjanto, T. R. Bieler, and D. Raabe. Overview of constitutive laws, kinematics, homogenization and multiscale methods in crystal plasticity finite-element modeling: Theory, experiments, applications. Acta Mater., 58(4):1152–1211, 2010. doi: 10.1016/j.actamat.2009.10.058.

[10] R. Asaro and A. Needleman. Overview no. 42 Texture development and strain hardening in rate dependent polycrystals. Acta Metall., 33(6):921–953, 1985. doi: 10.1016/0001-6160(85)90188-9.

[11] E. E. Nugent, R. B. Calhoun, and A. Mortensen. Experimental investigation of stress and strain fields in a ductile matrix surrounding an elastic inclusion. Acta Mater., 48(7):1451–1467, 2000. doi: 10.1016/S1359-6454(99)00444-9.

[12] M. Diehl, P. Shanthraj, P. Eisenlohr, and F. Roters. Neighborhood influences on stress and strain partitioning in dual-phase microstructures. Meccanica, 51(2):429–441, 2016. doi: 10.1007/s11012-015-0281-2.

[13] C. A. Bronkhorst, S. R. Kalidindi, and L. Anand. Polycrystalline Plasticity and the Evolution of Crystallographic Texture in FCC Metals. Philos. Trans. R. Soc. A Math. Phys. Eng. Sci., 341(1662):443–477, 1992. doi: 10.1098/rsta.1992.0111.

[14] P. Franciosi. Glide mechanisms in b.c.c. crystals: An investigation of the case of α-iron through multislip and latent hardening tests. Acta Metall., 31(9):1331–1342, 1983. doi: 10.1016/0001-6160(83)90044-4.

[15] S. Yadegari, S. Turteltaub, A. S. J. Suiker, and P. J. J. Kok. Analysis of banded microstructures in multiphase steels assisted by transformation-induced plasticity. Comput. Mater. Sci., 84:339–349, 2014. doi: 10.1016/j.commatsci.2013.12.002.

[16] J. W. Hutchinson. Bounds and Self-Consistent Estimates for Creep of Polycrystalline Materials. Proc. R. Soc. A Math. Phys. Eng. Sci., 348(1652):101–127, 1976. doi: 10.1098/rspa.1976.0027.

[17] J. C. Simo. Numerical analysis and simulation of plasticity. In P. G. Ciarlet and J. L. Lions, editors, Handb. Numer. Analys. vol. IV, 1998.

[18] T. Belytschko, W. K. Liu, and B. Moran. Nonlinear finite elements for continua and structures. 2009.

[19] J. C. Simo. On a fully three-dimensional finite-strain viscoelastic damage model: Formulation and computational aspects. Comput. Methods Appl. Mech. Engrg., 60(2):153–173, 1987. doi: 10.1016/0045-7825(87)90107-1.

[20] N. Vajragupta, V. Uthaisangsuk, B. Schmaling, S. Münstermann, A. Hartmaier, and W. Bleck. A micromechanical damage simulation of dual phase steels using XFEM. Comput. Mater. Sci., 54:271–279, 2012. doi: 10.1016/j.commatsci.2011.10.035.

[21] F. Maresca, V. G. Kouznetsova, and M. G. D. Geers. Subgrain lath martensite mechanics: A numerical-experimental analysis. J. Mech. Phys. Solids, 73:69, 2014. doi: 10.1016/j.jmps.2014.09.002.

[22] Y. Mine, K. Hirashita, H. Takashima, M. Matsuda, and K. Takashina. Micro-tension behaviour of lath martensite structures of carbon steels. Mater. Sci. Eng. A, 560:535–544, 2013. doi: 10.1016/j.msea.2012.09.099.
[23] D. L. Steinbrunner, D. K. Matlock, and G. Krauss. Void formation during tensile testing of dual phase steels. *Metall. Trans. A*, 19(3):579–589, 1988. doi: 10.1007/BF02649272.

[24] F. A. McClintock. A Criterion for Ductile Fracture by the Growth of Holes. *J. Appl. Mech.*, 35(2):363–371, 1968. doi: 10.1115/1.3601204.

[25] J. R. Rice and D. M. Tracey. On the ductile enlargement of voids in triaxial stress fields. *J. Mech. Phys. Solids*, 17(3):201–217, 1969. doi: 10.1016/0022-5096(69)90033-7.

[26] G. R. Johnson and W. H. Cook. Fracture characteristics of three metals subjected to various strains, strain rates, temperatures and pressures. *Eng. Fract. Mech.*, 21(1):31–48, 1985. doi: 10.1016/0013-7944(85)90052-9.

[27] T. W. J. de Geus, R. H. J. Peerlings, and M. G. D. Geers. Microstructural topology effects on the onset of ductile failure in multi-phase materials. A systematic computational approach. *Int. J. Solids Struct.*, 67-68:326–339, 2015. doi: 10.1016/j.ijsolstr.2015.04.035.

[28] J. R. Brockenbrough, S. Suresh, and H. A. Wienecke. Deformation of metal-matrix composites with continuous fibers: geometrical effects of fiber distribution and shape. *Acta Metall. Mater.*, 39(5):735–752, 1991. doi: 10.1016/0956-7151(91)90274-5.