Microscopic plasticity and damage in two-phase steels: On the competing role of crystallography and phase contrast

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A B S T R A C T

This paper unravels micromechanical aspects of metallic materials 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 at the meso-scale is unclear: is the plastic response dominated by the grain's anisotropy, or is this effect overwhelmed by the mechanical contrast between the two phases? The answer impacts the modeling of such a material at the meso-scale, but also gives insights in the resulting fracture mechanisms at that length-scale. Until now, this question has been addressed only for particular crystallographies and mechanical properties. In contrast, this paper studies the issue systematically using a large set of phase distributions, crystallographies, and material parameters. It is found that the macroscopic and the mesoscopic (grain-averaged) plastic response of the two extreme modeling choices (crystal plasticity or isotropic plasticity) converge with increasing phase contrast. The effect of the crystallography is completely overwhelmed by the phase contrast 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 the phases. The latter is quantified in this paper through the average arrangement of the phases around fracture initiation sites.

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1. Introduction

This paper studies the plastic response of two-phase metals that from an engineering perspective combine strength with ductility. The microstructure typically consists of two phases, a soft and a hard phase. We study the competition between plasticity due to the misalignment of the slip systems of the grains, and that due to the difference in slip resistance between the two phases. We aim to determine their relative influence on the plastic response at the meso-scale level (which has a grain-averaged resolution); showing that at that level the underlying physics may potentially be considered in an averaged sense. From a modeling point of view this implies that an isotropic plasticity model may provide sufficiently accurate predictions. Such a model is substantially simpler and computationally less expensive than the more realis-

tic crystal plasticity model. 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 reconciling apparently contradictory conclusions in different regimes.

In accordance with the considered grain-averaged quantities, an idealized microstructural morphology comprising equi-sized square grains is used. This offers the advantage of well controlled variations. Even more important is that the computations are relatively inexpensive as few finite elements suffice to discretize the microstructure accurately. For more targeted studies, involving only one or a few microstructures, such a simplification is not strictly needed and more realistic morphologies, in three dimensions, may be used (Zhao et al., 2008; Wong et al., 2015; Proudhon et al., 2016; Vachhani and Kalidindi, 2015; Delannay et al., 2006; Melchior and Delannay, 2006).

Materials that belong to the category of interest are metal-matrix composites and advanced high strength steels. The metal-matrix composites often have a (soft) aluminum matrix reinforced by (hard) silicon-carbide particles. It was recognized that in that

Nomenclature

$\langle\ldots\rangle$	ensemble average
$\bar{a}$	volume average
$\boldsymbol{A}$	second order tensor
$\mathbb{A}$	fourth order tensor
$\mathbb{C} = \boldsymbol{A} \otimes \boldsymbol{B}$	dyadic tensor product
$\boldsymbol{C} = \boldsymbol{A} \cdot \boldsymbol{B}$	single tensor contraction
$c = \boldsymbol{A} : \boldsymbol{B} = A_{ij}B_{ji}$	double tensor contraction

case 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 (Aghababaei and Joshi, 2011; Needleman and Tvergaard, 1993; McHugh et al., 1993; Nugent et al., 2000). 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 numerical studies were extended with more realistic microstructures (e.g. Choi et al., 2009; Sun et al., 2009; Kumar et al., 2006) but also with more realistic constitutive models, often involving crystal plasticity (e.g. Choi et al., 2013; Tjahjanto et al., 2006; Roters et al., 2010; Temizer, 2016; Maresca et al., 2016).

For single phase materials, the effects of crystallography on the plastic and damage response are significant, as the misalignment of grains introduces mechanical contrast (Asaro and Needleman, 1985). The natural question that arises is to what extent the phase contrast in two-phase materials dominates over 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 while the crystallography is less important (Needleman and Tvergaard, 1993; McHugh et al., 1993; Nugent et al., 2000). Although most studies are obviously numerical, Nugent et al., 2000 present an experiment in which rigid fiber is embedded in an analog matrix material (silver chloride). Local measurements using transmission electron microscopy were compared to isotropic elasto-plastic simulations. A satisfactory accuracy of the model predictions compared to the experiments was found except for observations with sub-grain resolution. For dual-phase steels, wherein also the hard phase deforms plastically, the crystallography appears to play an important role that may not be neglected (Choi et al., 2013; Diehl et al., 2016).

These studies were however mostly focused on the sub-grain response based on a specific set of crystallographies and 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 end. The analysis is extended to the initiation of fracture for which the outcome of the competition between crystallography and phase contrast is yet undetermined. In particular for this case, 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.

2. Microstructural model

2.1. Microstructure and spatial discretization

The microstructure is represented by an ensemble of 256 idealized periodic unit-cells, each made up of 32×32 equi-sized *grains* in which the phases are randomly distributed. An example unit-cell is shown in Fig. 1(a). Because we are interested in the *grain-averaged* (tensorial) quantities, the morphological idealization enables a relatively coarse numerical discretization, as discussed below.

Not the individual unit-cells but the ensemble as a whole is considered to be representative for the material. Accordingly, the hard phase volume fraction is set for the ensemble, but fluctuations are allowed between the individual unit-cells. 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, φ^{hard}. A reference value $\varphi^{\text{hard}} = 0.25$ is considered, resulting in unit-cells with hard phase volume fractions of $\varphi^{\text{hard}} = 0.25 \pm 0.04$. The crystallography of the grains is discussed in the next section.

A finite element based solution scheme is used, whereby each grain is discretized using 2×2 eight node bi-quadratic quadrilateral elements (see Fig. 1(b)), each of which is numerically integrated using four Gauss points. The quantities of interest are then averaged over the total of 16 Gauss points in each grain. A mesh convergence study has been performed to verify that, using the described discretization, the maximum relative error in terms of the considered quantities is lower than 2% with respect to a much finer discretization of 6×6 quadratic elements per 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 $\bar{\boldsymbol{F}}$. 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

$$\bar{\boldsymbol{\varepsilon}} = \frac{\sqrt{3}}{2} \, \bar{\varepsilon} \left(\vec{e}_x \vec{e}_x - \vec{e}_y \vec{e}_y \right) \tag{1}$$

where $\bar{\varepsilon}$ represents the equivalent logarithmic strain and $\vec{e}_x$ and $\vec{e}_y$ are the Cartesian basis vectors, respectively in horizontal and vertical direction. To introduce sufficient plastic deformation, $\bar{\varepsilon} = 0.2$ is used (applied in 2000 steps for 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