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Microstructural modeling of ductile fracture initiation in multi-phase materials

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ABSTRACT

The precise mechanisms underlying the failure of multi-phase materials may be strongly dependent on the material's microstructural morphology. Micromechanical modeling has provided much insight into this dependence, but uncertainties remain about crucial modeling assumptions. This paper assesses the influence of different grain shapes, damage indicators, and stress states using a structured numerical model. A distinct spatial arrangement of phases around fracture incidents is found, consisting of hard regions in the tensile direction interrupted by soft regions in the directions of shear. These key features are only mildly sensitive to the studied variations.

1. Introduction

Multi-phase materials, such as dual phase steel, metal matrix composites, etc., are frequently used in engineering applications. These materials often compromise strength with ductility. This favorable combination of properties is achieved by combining two or more phases at the level of the microstructure, for example hard (yet brittle) particles embedded in a soft (ductile) matrix. Although the macroscopic elasto-plastic and hardening behavior may be reasonably well predicted for a given microstructure [1–5], many uncertainties remain about the dominant failure mechanism(s). Experimental observations based on fractography, in situ electron scanning microscopy and tomography suggest that failure often occurs by ductile fracture of the, generally relatively soft, matrix phase [6–10]. However, also different mechanisms are observed in dual-phase steel [8,11,7,12], and in metal-ceramic composites in particular with a comparatively hard matrix phase [13,10].

Several numerical studies have been performed aiming to unravel the complexity of the fracture mechanisms. These models often use a relatively simple representation of the material in which the different phases are considered elasto-plastic, whereby fracture is associated with large local plastic deformation, see [1,14,2,15,16,5] and others. For example, Choi et al. [14] reported that lower levels of damage occur when the hard phase is distributed more homogeneously. Only few studies have performed a systematic analysis of the effect of the local phase distribution on failure. Kumar et al. [16] generated statistically representative microstructures from which a critical configuration is identified. This so-called "hot-spot" consists of a soft region neighbored on both sides by regions of the hard phase. It is often recognized that the local

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Nomenclature

$\boldsymbol{A}$	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
$\langle a \rangle$	ensemble average
$\bar{a}$	volume average
$\lfloor a \rfloor = \frac{1}{2}(a + \lvert a \rvert)$	positive part of a

incompatibility triggers both a high hydrostatic stress and high plastic deformation [17]. By combining a large number of different microstructures a similar observation was made by De Geus et al. [18], who identified the average phase distribution around the initiation of fracture. In addition to the observations by Kumar et al. [16] it was found the band of hard phase in the tensile direction is interrupted by a band of soft phase in the direction of maximum shear.

From a modeling point of view different approaches are used to incorporate and/or study the micromechanics of a two-phase material. Unit cell models have been used to study the basic micromechanical response, including fracture initiation mechanisms [19–22]. To accommodate the geometrical complexity of two- or multi-phase materials, models are needed that include a large number of particles/grains. Models that are based on a real microstructure with all geometrical details, however, suffer from a large number degrees-of-freedom. Furthermore, it is difficult to apply systematic variations in terms of composition and morphology, without changing other parameters at the same time, to unravel their influence on fracture initiation. Therefore, structured models consisting of square elements are frequently used (e.g. [16,18]). Moreover, the numerical complexity is often reduced by using simplified damage indicators (e.g. [1,14,2,15,16,5,18]). It is not trivial to assess how the resulting conclusions are influenced by the approximations made therein.

In particular, in our earlier work [18], a microstructure of square equi-sized grains was employed in combination with a simple indicator for fracture initiation, which was based on the well known fact that ductile fracture takes places when a combination exists of a high hydrostatic tensile stress and high plastic deformation. The particular interest was to study which characteristic features in the two-phase microstructure give rise to such conditions. The main finding was that initiation of fracture is strongly governed by the local arrangement of the two phases. A critical arrangement was identified by calculating the average phase distribution around the critical site. It remains, however, questionable to what degree the main conclusions depend on the aforementioned assumptions. The current contribution aims to remedy this concern, by a critical assessment of the effect of the assumptions on the critical phase distribution around fracture initiation. For this purpose, the following analysis steps are made:

1. The basic, Rice & Tracey-like damage indicator is replaced by a more involved Johnson–Cook damage indicator.
2. The square cells used to represent the individual phases are compared to hexagonal cells, in which (in contrast to the squares) the phases are never connected by a single point.
3. The applied pure-shear deformation is extended with a volumetric contribution to consider different strain paths resulting in different stress states, which remain proportional throughout the deformation history.

Like in [18], this study is limited to the initiation of ductile fracture in the matrix phase, initiation of fracture in the hard phase and in the interface between the hard and the soft phase are not considered. Furthermore, fracture propagation is not considered.

This paper is structured as follows: the microstructural model, including a summary of the main conclusions of [18], is discussed in Section 2. The influence of the respective assumptions are separately discussed in Sections 3–5, followed by a discussion and a summary of the conclusions in Section 6.

2. Reference model and summary of earlier results

This section describes the model and summarizes the main conclusions reported in [18]. Several parts of the model are slightly modified, whereby the most important difference is the adopted three-dimensional discretization to allow for more general stress states. Furthermore, the composition of the microstructure is resolved in a weak sense, only allowing fluctuations in the individual microstructural volume elements in the ensemble, as discussed below. The presented results are all generated with the model presented here.