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Integrated experimental–simulation analysis of stress and strain partitioning in multiphase alloys

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Abstract

The mechanical response of multiphase alloys is governed by the microscopic strain and stress partitioning behavior among microstructural constituents. However, due to limitations in the characterization of the partitioning that takes place at the submicron scale, microstructure optimization of such alloys is typically based on evaluating the averaged response, referring to, for example, macroscopic stress–strain curves. Here, a novel experimental–numerical methodology is introduced to strengthen the integrated understanding of the microstructure and mechanical properties of these alloys, enabling joint analyses of deformation-induced evolution of the microstructure, and the strain and stress distribution therein, down to submicron resolution. From the experiments, deformation-induced evolution of (i) the microstructure, and (ii) the local strain distribution are concurrently captured, employing in situ secondary electron imaging and electron backscatter diffraction (EBSD) (for the former), and microscopic-digital image correlation (for the latter). From the simulations, local strain as well as stress distributions are revealed, through 2-D full-field crystal plasticity (CP) simulations conducted with an advanced spectral solver suitable for heterogeneous materials. The simulated model is designed directly from the initial EBSD measurements, and the phase properties are obtained by additional inverse CP simulations of nanoindentation experiments carried out on the original microstructure. The experiments and simulations demonstrate good correlation in the proof-of-principle study conducted here on a martensite–ferrite dual-phase steel, and deviations are discussed in terms of limitations of the techniques involved. Overall, the presented integrated computational materials engineering approach provides a vast amount of well-correlated structural and mechanical data that enhance our understanding as well as the design capabilities of multiphase alloys.

Keywords: In situ testing; Digital image correlation; Crystal plasticity; Spectral method; Dual-phase steel

1. Introduction

Simultaneous improvement of material strength and ductility is achievable by microstructures that combine several deformation and strengthening mechanisms. With the exception of single-phase materials showing deformation-dependent transitions between different strain-hardening mechanisms (*e.g.* twinning-induced plasticity (TWIP) steels [1]), in current alloy design practice joint strength and ductility optimization is typically realized by introducing different phases with contrasting mechanical characteristics. Recent examples of such systems are dual-phase (DP, [2,3]), transformation-induced plasticity (TRIP, [4,5]) steels, and $(\alpha+\beta)$-Ti-alloys [6,7], etc.

The phase-specific deformation or transformation mechanisms present in such microstructures are triggered at different local stress or strain levels, and, therefore, the global performance of such alloys under mechanical loading critically depends on the evolution of stress and strain partitioning among the different phases. Thus, to understand the behavior of existing high-strength alloys and to

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design new composites, phases and interfaces with improved properties, analysis of the microstructural strain and stress partitioning is crucial [8]. Moreover, to identify physically based microstructure design guidelines, it is essential that the measurement of strain and stress fields is further coupled to the measurement of the deformation-induced evolution of the underlying microstructure itself. The concurrent mapping of strain, stress and microstructure-evolution, however, is highly challenging since:

i. mapping of the deformation-induced evolution of such complex microstructures requires the use of microscopy techniques that provide excellent phase and defect contrast at both high resolution and large field of view;
ii. mapping of microscopic strain fields requires a high-performance microscopic-digital image correlation (μDIC) methodology that does not suffer from limited resolution/field-of-view, patterning-induced microstructure modification, and inaccuracies at high strain levels [9–14];
iii. mapping of microscopic stress fields at the required spatial resolution is challenging by stand-alone experiments, calling for complementary crystal mechanics simulations.

In the literature, the mapping of these three different "fields" has typically been achieved through experimental in situ techniques (e.g. [1,3,4,15–18]) or by numerical simulations [19–23], in an uncoupled manner. Among the experimental approaches, earlier works focused on basic mapping of microstructure evolution (based on topographic trace analysis) without strain mapping [16] or subsequently on mapping macroscopic strain fields without coupling to the underlying microstructure evolution [17,24]. Most recent efforts following the introduction of μDIC include mapping of microscopic strain fields together with some basic (*i.e.* topography-based) analysis of microstructure evolution [14,15,25,26]. A more direct coupling between μDIC and the underlying microstructure is obtained through accompanying electron backscatter diffraction (EBSD) measurements in Ref. [27]. Among the simulation efforts, the great majority of early works were based on morphologically simplified unit cell models [20,22,23,28]. In the recent years, crystal plasticity (CP) finite-element method (FEM)-based numerical analyses were increasingly based on experimentally obtained microstructure maps [19,29–38]. This trend is expected to further develop and include an increasing level of microstructural authenticity and detail (e.g. [37,38]). There are, however, only few very recent examples [39,40] that aim to couple the deformation-induced microscopic strain or stress field evolution to the experimental analysis of the deformation of the same starting microstructure. A number of technical challenges have hampered the interactions between experiments and simulations so far, and thus more holistic approaches to couple advanced experimental and simulation tools and methodologies in an integrated manner are required to match the three requirements (i)–(iii) described above.

In this work we present a novel, integrated experimental–numerical methodology that fulfills these conditions, allowing concurrent analysis of deformation-induced evolution of microstructure, strain partitioning and stress partitioning. With this methodology, as shown schematically in Fig. 1, the first is derived from experiments and the last from the corresponding CP simulations, while the strain mapping is obtained from both. In the experiments, to allow strain and microstructure mapping (*i.e.* challenges (i) and (ii) above), a recently developed μDIC technique is employed that provides high-resolution (approximately 0.1 ± 0.001 μm) strain maps without inhibiting the application of EBSD measurements, electron channeling contrast imaging (ECCI) [41] and secondary electron (SE) imaging measurements of the same microstructural region [10]. The simulation route also starts from the EBSD map of the same area (Fig. 1), from which a crystallographically informed numerical model is created with phase properties obtained from inverse CPFEM simulations of nanoindentation experiments [42,43]. Using a recently developed spectral solver suitable for heterogeneous materials with high mechanical phase contrast and nonlinear stress–strain response [44,45], full-field CP simulations are carried out. Guided by a comparison with the experimentally obtained strain fields, these simulations allow mapping local stress fields, thus providing an indirect solution for challenge (iii) described above.

Here we demonstrate the potential of the methodology on the example of a DP steel, which is an ideal case study material for stress and strain partitioning due to the coexistence of the high mechanical contrast phases martensite and ferrite with comparable volume fractions. First, a detailed explanation of the experimental and numerical methods is provided, followed by results obtained from both routes in a consecutive manner. These results are then analyzed and discussed in direct comparison, focusing on various phenomena that are characteristic for DP steel micromechanics.

2. Methodology

The strength of the methodology lies in the strong coupling between experiment and modeling as schematically outlined in Fig. 1. In this section, the methodologies followed in both routes are explained in detail, referring to Figs. 2 and 3, respectively.

2.1. In situ experiments

For the experiments, tensile samples with gauge dimensions of 4 mm × 2 mm × 1 mm are produced by spark erosion. Specimen surfaces are polished with colloidal SiO_2 particles ranging from 0.01 to 0.05 μm in size, following a conventional metallographic grinding, diamond polishing and etching procedure. Preliminary large field-of-view