Materials Science & Engineering A 695 (2017) 101–111

Contents lists available at ScienceDirect

Materials Science & Engineering A

journal homepage: www.elsevier.com/locate/msea

An RVE procedure for micromechanical prediction of mechanical behavior of dual-phase steel

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ARTICLE INFO

Keywords:
Crystal plasticity
Dual phase steel
Representative volume element
Dislocation pile-up
Superdislocation

ABSTRACT

A "bottom-up" representative volume element (RVE) for a dual phase steel was constructed based on *measured* microstructural properties ("microproperties"). This differs from the common procedure of inferring *hypothetical* microproperties by fitting to macroscopic behavior using an assumed micro-to-macrolaw. The bottom-up approach allows the assessment of the law itself by comparing RVE-predicted mechanical behavior with independent macroscopic measurements, thus revealing the nature of the controlling micromechanisms. An RVE for DP980 steel was constructed using actual microproperties. Finite element (FE) simulations of elastic-plastic transitions were compared with independent loading-unloading-loading and compression-tension experiments. Constitutive models of three types were utilized: 1) a standard continuum model, 2) a standard Crystal Plasticity (CP) model, and 3) a SuperDislocation (SD) model similar to CP but including the elastic interactions of discrete dislocations. These comparisons led to following conclusions: 1) While a constitutive model that ignores elastic interaction of defects can be fit to macroscopic or microscopic behavior, it cannot represent both accurately, 2) Elastic interactions among dislocations are the predominant source of nonlinearity in the nominally-elastic region (i.e. at stresses below the standard yield stress), and 3) Continuum stress inhomogeneity arising from the hard martensite / soft ferrite microstructure has a minor role in the observed transitional nonlinearity in the absence of discrete dislocation interactions.

1. Introduction

Hill [1] introduced the idea of a representative volume element ("RVE") as a material sub-domain or cell to represent the microstructure of an alloy in a periodic or average sense. This "original-RVE[1]" concept was later transformed, effectively divorcing its properties from those of real microstructures and real microproperties.[2] As a well-known example of this "new-RVE" approach, hypothetical void arrays were constructed [2] that employed an assumed void volume fraction, typically much larger than any observed one (e.g. [3–5]). The "void fraction" thus morphed into an arbitrary internal variable in a micro-to-macro law, i.e. a model parameter in a constitutive model to allow micro-motivated FE simulation. Development of related new-RVE models [6,7] led to the field of "damage mechanics" [8–10]. It represents a fundamental shift away from the original-RVE concept.

When it is successful in application, the new-RVE procedure has merit for analyzing macro-scale problems. However, there is no assurance that an RVE constructed in such a reverse way has any

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[1] The term "RVE" is used in this work for any element representing microstructural morphology and properties, whether the properties are determined from macroscopic mechanical tests and simulation ("new-RVE") or by directly-measured morphology and properties ("original-RVE"). The two RVE's may generally look the same, but as discussed may have widely varying phase properties depending on how they are obtained. Both may be useful, but not unless their limitations are taken into account in reaching conclusions.

[2] The term "microproperty" is used here to designate the various single-crystal properties of each microstructural phases that determine its mechanical behavior: volume fraction, morphology, grain size, dislocation density, chemical composition, and strain hardening law. "Measured (or actual, or real) microproperties" denotes properties obtained from measurements corresponding to the individual grain and/or phase; this is in the spirit of the original RVE approach. "Back-fit (or hypothetical) microproperties" denotes properties obtained by assuming a law connecting micro- and macrobehavior, performing a macrotest, such as a tensile test, then performing a reverse analysis to obtain a set of hypothetical microproperties that are consistent with the assumed law and the measured macrobehavior. As will be shown, the micro- and macroproperties obtained in these alternate ways differ significantly, thus calling into question the accuracy of the connection law.

http://dx.doi.org/10.1016/j.msea.2017.04.032
Received 14 February 2017; Received in revised form 5 April 2017; Accepted 7 April 2017
Available online 09 April 2017
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Nomenclature

$\sigma_{Composite}$	flow stress of a fiber composite
σ_f	flow stress of fiber
σ_m	flow stress of matrix
V_f	volume fraction of fiber in the composite
σ_y	yield stress with no particle
α'	constant on the order of unity in Orowan equation (Eq. (2))
L	particle spacing
σ_0	frictional stress
k_y	material constant in Hall-Petch equation (Eq. (3))
M	Taylor factor
k	material constant related to dislocation character
τ_{obs}	obstacle strength
μ	shear modulus
b	Burgers vector
d	grain size
E	Young's modulus
υ	Poisson's ratio
K	strength material constant
$\overline{\varepsilon_0}$	constant that may represent a pre-strain
n	strain hardening exponent
$\tau^{(\alpha)}$	resolved shear stress on the αth slip system
$\dot{\gamma}_0$	reference shear rate
m	strain rate sensitivity
$g^{(\alpha)}$	slip resistance on the slip system α
$g_0{}^{\alpha}$	initial slip resistance on the slip system α
τ_b	back-stress
$\rho^{(\alpha)}$	dislocation density in slip system α
$\boldsymbol{h}_{\alpha\beta}$	interaction cosine
$n^{(\alpha)}$	slip plane normal of slip system α
$\boldsymbol{\xi}^{(\beta)}$	dislocation line vector of slip system β
A	material constant in slip resistance equation (Eq. (7))
k_a	material constant related to dislocation generation
k_b	material constant related to dislocation annihilation
$\dot{\rho}^{(\alpha)}_{pass}$	rate of dislocation density passing through the element
$l^{(\alpha)}$	length of the element parallel to the slip plane α
τ^*	maximum obstacle strength
N	geometrical transmissivity factor
L_1,L_i	intersection line vectors between grain boundary and slip planes
s_1,s_i	slip direction vectors of incoming and transmitted dislocations of incoming and transmitted dislocations
E_T	instant tangential modulus
$\Delta\varepsilon$	absolute value of strain change after load reversal
$\Delta\sigma$	absolute value of stress change after load reversal

connection to the real microstructure or microproperties. The procedure instead convolutes two aspects: 1) hypothetical microproperties and 2) assumed micro-to-macroconstitutive model. Only the combined pair has validity: the two cannot be separated to obtain meaningful independent components.[3] Clearly the procedure cannot be used to identify or confirm the microscopic mechanism controlling the macroscopic behavior, although many published results purport by inference to do this.

1.1. Scale-free methods

The mechanical strength and stability of composite materials [11] has been interpreted using the new-RVE approach. Examples have been presented for elastic properties [12–14], elastic-plastic properties [15,16], and cyclic behavior at room temperature [17] and at elevated temperature [18]. A key assumption inherent in such approaches is that the scale of the governing material structure is sufficiently coarse that discrete defect interactions can be ignored without large errors.

When the assumption is valid, the methods can produce accurate predictions without complex adjustments. For example, rule-of-mixtures models adequately predicted tensile strength and elongation of a steel [29] and metallic composites [30]. Such methods rely on a relationship of the following type [31]:

$$\sigma_{composite} = V_f\sigma_f + (1 - V_f)\sigma_m \quad (1)$$

where $\sigma_{Composite}$, σ_f and σ_m are the flow stress of a fiber composite, fiber, and matrix, respectively and V_f is the volume fraction of fiber in the composite. Matlock and Speer [32,33] concluded that such models reproduced DP steel behavior properly, whereas Orowan models were not considered to be of practical interest. The accuracy of this conclusion is a major question to be addressed herein.

Scale-free RVE models take into account the morphology of the microstructure, but not its scale. Recently, such models have been applied to DP steels [26–28,43–51]. In most of these, the “new-RVE” approach sets the microproperties from macroscopic data, either directly (i.e. inferring constituent strength from composite strength) [44] or indirectly (constructing and/or using a strength-vs.-chemical composition map from macroscopic measurements) [26-28,43,45–47].

In order to reproduce known macroscopic properties of DP steels, the martensite phases are typically assigned unrealistic ultimate tensile strengths (UTS). For example, Ha et al. [43] set the martensite UTS at 2500 MPa in a DP590 steel, while 1400 MPa is expected based on direct measurements for the reported carbon concentration [52]. Similarly, Govik [44] applied a new-RVE scheme to “predict” nonlinear elastic-plastic transitions in a DP600 steel. However, the results shows that the assigned UTS of the martensite is even higher than that in Ha et al., at 2600 MPa. Such strengths are not consistent with any direct measurement of martensite phases of a similar composition. In fact, Govik's result tends to contradict his conclusion about identifying the proper micro-mechanism governing the nonlinearity.

New-RVE modeling for DP steel has also been performed using CP methods [53,54], rather than the purely continuum models [43,44]. However, the microproperties were again reverse-engineered from macroscopic results and continue to ignore microstructural scales.

1.2. Well-established scale effects

Scale-free models ignore well-known scale effects, for example Orowon's mechanism, or its so-called “hard pin” variation [34,35]

$$\sigma = \sigma_y + \alpha'\mu b/L \quad (2)$$

where σ_y is the yield stress with no particle, α' is a constant on the order of unity, L is the spacing between particles, i.e. a measure of microstructural scale, μ is the shear modulus and b is the burger's

[3] An easily-understood example of this distinction is the ubiquitous “texture analysis” performed based on a single crystal plasticity constitutive model (e.g. the PAN model [63,64,103]) taking into account a statistical distribution of slip system orientations representing all of the grain orientations in an average and smoothed sense. The microproperties are inferred from macroscopic tests, e.g. tensile tests. Such a model has value in that it can predict texture-related plastic anisotropy, which relies on this scale-free average orientation. However, the inferred micro-properties have little or no connection with actual microproperties such as flow strength. That this is true can easily be seen by noting that the strength of the polycrystal can vary by an order of magnitude or more by changing the grain size alone via the Hall-Petch effect [36,37]. This change occurs with no change of the real microproperties, but in the combined model that difference of strength is attributed to spurious variation of strength of the single crystals in the single crystal constitutive model. Therefore, the final model, no matter how useful, represents neither a microstructurally-based RVE, nor a constitutive model for the constituents, as has been shown recently [60–62].

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