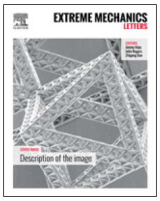
Extreme Mechanics Letters 13 (2017) 36–41

Contents lists available at ScienceDirect

Extreme Mechanics Letters

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



Size affected dislocation activity in crystals: Advanced surface and grain boundary conditions

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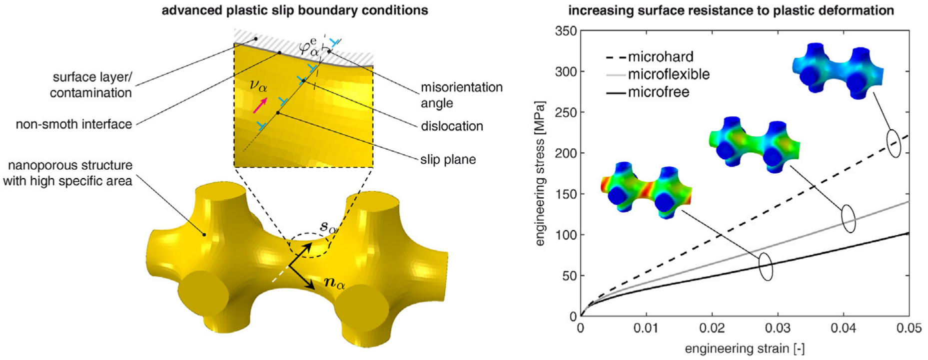
GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 14 October 2016
Received in revised form
20 December 2016
Accepted 19 January 2017
Available online 23 January 2017

Keywords:
Higher-order boundary conditions
Gradient extended crystal plasticity
Defect density
Size effect
Surface yielding
Nanoporous gold

ABSTRACT

Extended crystal plasticity theories are well established to study size-dependent hardening of metals. Surface and inner grain boundary conditions play a significant role for crystals at small scales as they affect the dislocation activity and, hence, alter strength and strain hardening behavior. Conventional micro boundary conditions, i.e., microhard and microfree, are unable to capture the underlying physics as they describe ideal and over-simplified surface/interface conditions. In this work, advanced boundary conditions for gradient extended crystal plasticity are introduced to map realistic conditions at external surfaces, interphases, or grain boundaries. They relate the magnitude of plastic slip to surface defect density and slip directions with respect to the surface normal. Characteristic features are highlighted, including the effect of surface yielding and size dependent surface strengthening.

1. Introduction

In crystalline solids, perfect crystalline behavior ceases to exist near external surfaces, grain boundaries between two crystals of the same phase and interphase boundaries between two different phases [1,2]. Since the binding of an atom to its neighbors contributes a negative term to the energy of a crystal, Gibbs free energy at these surfaces is modified due to inhomogeneities at the nanoscale, such as altered bonds. This difference in bonding as compared to the bulk generally causes an extra surface stress [3]. Dislocation dynamics and, thus, macroscopic plastic behavior is also influenced by the presence of a surface to create size effects on

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http://dx.doi.org/10.1016/j.eml.2017.01.007

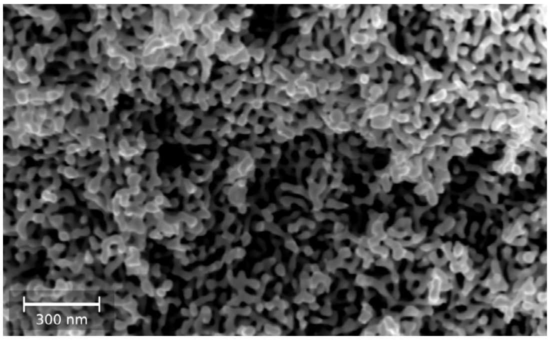

Fig. 1. Scanning electron micrograph of nanoporous gold with an exceptionally high surface-to-volume ratio.
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yield stress and work hardening. The surface's influence becomes substantial once the number of atoms sitting at the surface relative to those lying within the bulk increases, e.g., in the case of ultrafine-grained metals, thin films, nanoporous materials [4].

With its nanoscale porosity and high specific surface area, nanoporous gold demonstrates extreme chemo-mechanical activity [5]. Its catalytic activity, electrical conductivity, morphological properties (e.g., high specific surface area), and mechanical properties (e.g., reduced stiffness), make nanoporous gold attractive in numerous applications such as actuation, catalysis, sensors and microfluids [5–7]. In nanoporous gold the load bearing structure is a network of ligaments (cf. Fig. 1) with diameters of 5 nm to several micrometers, depending on the post annealing treatment [8–10]. Although brittle in tension, nanoporous gold shows considerable malleability, that is, extreme ductility under compressive stress in the vicinity of crack tips with ligaments occasionally strained by as much as 200% [11,12]. Microscopic characterization of fracture surfaces indicated that dislocation activity is suppressed in nanoscale ligament structures while dislocation activity is present in heat treated nanoporous gold with average ligament diameter of $\approx 1\ \mu\text{m}$ [11]. In addition to the effect of suppressed dislocation nucleation [13], emission and reabsorption of dislocations at free surfaces is another source of size dependent hardening [14].

In this work, we study the plastic[1] deformation behavior of nanoporous gold in the context of gradient extended crystal plasticity at finite strains. The focus is on novel higher-order boundary conditions reflecting microscopically non-idealized conditions at external surfaces, grain boundaries, or interfaces. In the vast majority of analytical and numerical studies, two types of simple, idealized boundary conditions are adopted, namely microfree and microhard. The former characterizes conditions with vanishing micro-stresses, i.e., no microscopic force conjugated to geometrically necessary dislocations (GNDs) occurs as a driving force on the body. Dislocations are free to escape at the surface, hence no dislocation pile-ups occur. At the other extreme, i.e., for microhard conditions, plastic slip vanishes at the boundary, preventing any dislocation escape.

Non-idealized boundary conditions are of interest, for instance, if the exterior causes additional resistance to plastic deformation or, in other words, if dislocations are not enabled to move unrestricted through the surface. Related discussions, including size effects on the yield stress and work hardening as well as the impact of surface effects on fracture properties, are found in [16]. Oxidation on nanoporous gold films[2] is higher than on planar gold due to increased catalytic activity of the porous network [20,21]. Buckley [17] demonstrated that thin films on the surface of single crystal Au increased the surface hardness. This was attributed to increased resistance to plastic deformation by the impeded escape of dislocations by the presence of the oxide film, referred to as the Roscoe effect [22].[3] Therefore, mechanical properties of small-scaled samples are related (to some extent) to their surfaces.

Although highly relevant, this aspect of dislocation-surface interaction modeling has not been studied in the literature for nanoporous gold. With this work, we attempt to bridge this gap by presenting computational modeling of advanced higher-order boundary conditions for Au single crystals. As a demonstrative example, their impact on the deformation response of a periodic nanoporous Au microstructure is examined. The chosen geometry is characterized by a typical microstructural feature with curved surfaces frequently found in nanoporous metals. This results in many diverse misorientation angles.

Grain boundary conditions, i.e., inner boundaries in polycrystals, which are physically more meaningful than their idealized counterparts have been studied by [24–29]. Only very few works are devoted to a computational framework for surface effects in single crystals. In these, the formation of surface steps during plastic deformation is taken as an additional source for size-dependent hardening and strengthening [30,31]. The conditions proposed in this work are more general and capable of modeling a wide range of dislocation-surface interactions.

2. Gradient extended single crystal plasticity

2.1. Basic relations

The thermodynamic consistent framework for gradient-enhanced crystal plasticity is recalled based on [32]. The large deformation theory is employed in terms of the multiplicative decomposition of the deformation gradient $\boldsymbol{F} = \boldsymbol{F}_{\mathrm{E}} \cdot \boldsymbol{F}_{\mathrm{P}}$, where $\boldsymbol{F}_{\mathrm{E}}$ is the pure elastic and $\boldsymbol{F}_{\mathrm{P}}$ the plastic deformation part. As usual, this motivates the right Cauchy–Green stretch tensors $\boldsymbol{C} = \boldsymbol{F}^{\mathrm{T}} \cdot \boldsymbol{F}$ and $\boldsymbol{C}_{\mathrm{E}} = \boldsymbol{F}_{\mathrm{E}}^{\mathrm{T}} \cdot \boldsymbol{F}_{\mathrm{E}}$. Furthermore, the first and second Piola–Kirchhoff stress denoted as $\boldsymbol{P}$ and $\boldsymbol{S}_{\mathrm{E}}$, respectively, are of interest. The relation between these stress measures is given by $\boldsymbol{P} = \boldsymbol{F}_{\mathrm{E}} \cdot \boldsymbol{S}_{\mathrm{E}} \cdot \boldsymbol{F}_{\mathrm{P}}^{-\mathrm{T}}$. For the particular choice of a Neo-Hookean hyperelastic material behavior, the second Piola–Kirchhoff stress yields

$$\boldsymbol{S}_{\mathrm{E}} = \mu \boldsymbol{I} + [\lambda \ln(J) - \mu]\, \boldsymbol{C}_{\mathrm{E}}^{-1}, \tag{1}$$

where $J = \det(\boldsymbol{F}_{\mathrm{E}})$ is the Jacobian determinant; μ and λ denote the Lamé parameters. Moreover, the Mandel stress is introduced as $\boldsymbol{M}_{\mathrm{E}} = \boldsymbol{C}_{\mathrm{E}} \cdot \boldsymbol{S}_{\mathrm{E}}$ – the work conjugate to the plastic velocity gradient $\boldsymbol{L}_{\mathrm{P}} = \dot{\boldsymbol{F}}_{\mathrm{P}} \cdot \boldsymbol{F}_{\mathrm{P}}^{-1} = \sum_{\alpha} \nu_{\alpha} [\boldsymbol{s}_{\alpha} \otimes \boldsymbol{n}_{\alpha}]$ which is defined via plastic slip rates ν_{α} on corresponding slip planes $\boldsymbol{s}_{\alpha} \otimes \boldsymbol{n}_{\alpha}$. In this respect, the crystallographic geometry of each slip system α is specified in terms of slip direction $\boldsymbol{s}_{\alpha}$, slip plane normal $\boldsymbol{n}_{\alpha}$, and transverse slip direction $\boldsymbol{t}_{\alpha} = \boldsymbol{n}_{\alpha} \times \boldsymbol{s}_{\alpha}$. It is further assumed that plastic deformation is lattice preserving.

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[1] The influence of surfaces on the elastic behavior is studied in another work; elastic and plastic Poisson's ratios of nanoporous gold were investigated experimentally and numerically in [15].

[2] At temperatures less than 900 °C gold does normally not form a stable oxide in air or oxygen [17,18]. However, electrochemical techniques allow generation of oxides on gold surface [19].

[3] This scenario is not limited to gold. It is demonstrated in [23] that, on the course of deformation the oxide films in aluminum causes formation of a layer of edge dislocation dipoles trapped beneath the surface and reduction of the amount of surface slip. This reduction is observed to be larger for the increased oxide coating thickness. Hence, the proposed methodologies in this work have a wide range of applications although the current application is concentrated on the nanoporous gold.