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Computational modeling of intrinsically induced strain gradients during compression of *c*-axis-oriented magnesium single crystal

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Abstract

A finite-deformation strain gradient crystal plasticity model is implemented in a three-dimensional finite-element framework in order to analyze the deformation behavior and the stress–strain response of magnesium single crystals under *c*-axis orientation. The potential-based and thermodynamically consistent material model is formulated in a non-local and non-linear inelastic context in which dislocation densities are introduced via plastic strain gradients. Experiments have shown that the internal length scale of the microstructure starts to affect the overall stress–strain response when the sample size decreases to the micron scale. As a consequence, strain gradients develop, leading to an additional energetic-like hardening effect which results in an increase of the macroscopic strength with decreasing crystal size. In the case of uniaxial compression of *c*-axis-oriented single-crystal micropillars, the model is able to predict the discrete dislocation glide in terms of a band-shaped slip zone. Two different pillar sample sizes are taken into account in order to investigate the intrinsic size effect during plastic deformation where the crystallographic orientation leads to the activation of pyramidal $\{11\bar{2}2\}$ $\langle 11\bar{2}3\rangle$ slip systems as reported in various experimental studies. The interaction of those slip systems is expressed in terms of latent hardening and excess dislocation development. A comparison between numerical results and corresponding experimental data is presented.

Keywords: Strain gradient crystal plasticity; Geometrically necessary dislocations; Magnesium single crystal; Microcompression; Slip band

1. Introduction

Alternative lightweight materials such as magnesium will become more important in the future. Due to its low density and high strength-to-weight ratio, magnesium offers great potential for a wide range of applications. Especially in high-tech functional materials, fundamental knowledge of the microstructure is required to optimize the performance. The hexagonal close-packed (hcp) lattice structure of magnesium still represents a major challenge since its deformation behavior is more complex compared to that of face-centered cubic (fcc) metals. For that reason, a wide range of experimental studies has been performed in order to obtain a better understanding of the deformation mechanisms and their impact on the macroscopic strength. In this regard, small volume investigations using single crystals are performed under specific boundary conditions by which unwanted micromechanical processes can be excluded in order to focus on a particular deformation mechanism such as non-basal slip activation. Beside basal slip in hcp materials, the investigation of non-basal slip is of great interest since its impact on mechanical properties must be considered in the material design process. Essential for the activation of non-basal slip systems in single crystals is the crystallographic orientation with respect to the loading direction by which basal slip has no resolved shear

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stress, e.g. loading parallel [1,2] or perpendicular [3,4] to the basal plane.

Apart from slip activation, the material response is strongly influenced by the size of the sample if dimensions are reduced to the micrometer range. In the literature, different kinds of size effects have been observed. To this extent, an extensive review with respect to different crystalline and amorphous metals is provided by Greer and De Hosson [5]. A meaningful distinction of size-dependent strengthening effects was illustrated by Sevillano [6,7]. Here, size effects are classified into two types. According to Sevillano, extrinsic size effects are characterized by externally imposed plastic strain gradients, which are resolved by the storage of geometrically necessary dislocations (GNDs) [8–10]. As a consequence of the GND storage, size-dependent work hardening becomes significant if the gradient in plastic slip is significant or equivalently if the deformation length-scale is small relative to the distributed plastic strain. Typical examples for deformation length-scales are the penetration depth in micro- and nanoindentation tests [11,12], the beam thickness in microbending tests [13], and the wire diameter in microtorsion tests [10]. In particular, the storage of GNDs causes an additional energetic-like hardening effect which increases the macroscopic strength with decreasing sample size. Since such length scale-dependent hardening is not mapped by conventional crystal plasticity theory, a great variety of strain gradient crystal plasticity models have been developed. In those, the strain gradient is introduced into the mathematical model and, in many cases, associated with GNDs. Large deformation strain gradient crystal plasticity models have been formulated by a number of researchers (e.g. [14–20]). In contrast to extrinsic size effects, intrinsic size effects do not require the presence of mesoscopic plastic strain gradients but rather result from the interference of a plastic process zone with any internal (microstructural) length-scale [6], such as the average interdislocation distance, the interparticle distance or the physical size limited by free surfaces.

This paper aims at the computational modeling of *c*-axis-oriented magnesium single crystal where strain gradients are imposed intrinsically, due to the small sample size and the large microstructural length associated with the low dislocation density, single-crystalline structure. For this purpose, a finite-deformation strain gradient crystal plasticity model is implemented into a three-dimensional finite-element framework. While there have been several numerical studies of microcompression of fcc single crystals, to the authors' knowledge no such studies have been applied to hcp systems. For instance, Raabe and Roters [21] investigated the effect of different initial crystal orientations, diameter-to-height ratios and friction coefficients on the deformation behavior of copper single crystals using conventional crystal plasticity. In the work of Shade et al. [22], the lateral constraint effects of single-slip-oriented nickel-base superalloy single crystals were studied, also using conventional crystal plasticity. It turned out that the lateral constraint has a significant effect on the strain-hardening behavior. However, in both studies, the effects of GND-induced plastic slip gradients as described by Nye [8] were not considered. For this reason a deformation mode typically observed in microcompressed single crystals, which is characterized by a localization of several slip systems, cannot be reproduced. Recently, Kuroda [23] presented a numerical example using a strain gradient theory that is based on the same single-slip oriented nickel-base superalloy as investigated in Ref. [22]. It has been shown that the consideration of the gradient effect is essential for the formation of a particular deformation mode which is composed of a band-shaped slip zone and two dead zones. In this context, the study showed how various parameters, such as different macroscopic and microscopic boundary conditions as well as different length-scale to pillar diameter ratios, influence the deformation mode. In delimitation to this, we are focusing on a specific set of parameters in order to validate the here-applied strain gradient crystal plasticity model according to micromechanical testing of magnesium single crystal. The resulting stress–strain curves of two representative sample sizes are directly related to the experimental data of Lilleodden [24]. In addition, multiple slip, including slip system interactions in terms of latent hardening and latent dislocation nucleation resistance, is considered.

2. Micromechanics of single-crystal magnesium under *c*-axis compression

Due to its hcp crystal structure, crystallographic slip in magnesium primarily occurs on the (0001) basal plane where the close-packed slip directions are of type $\langle 11\bar{2}0\rangle$. However, many experimental observations have shown that non-basal slip takes place, especially if the loading direction is parallel or perpendicular to the basal plane. In this contribution, the relevant crystallographic orientation of magnesium single crystal is the *c*-axis- or (0001)-orientation as illustrated in Fig. 1. Note that the direction of the *c*-axis is coincident with the direction of the ⟨c⟩ Burgers vector, and is aligned with the loading axis of the indenter. Consequently, slip systems including the ⟨a⟩ Burgers vector, such as the basal slip systems have zero Schmid factor, i.e. they have no resolved shear stress. Therefore, those slip systems cannot contribute to a vertical deformation along the *c*-axis necessitating the activation of less easily activated slip systems. As reported first by Obara et al. [3] and Stohr and Poirier [4], pyramidal $\{11\bar{2}2\}\,\langle 11\bar{2}3\rangle$ slip, hereafter referred to as $\pi 2$ slip, was observed during compression tests of magnesium single crystal along the *c*-axis. Due to the symmetry along the *c*-axis, six $\pi 2$ slip systems are exposed to the same stress. The simultaneous activation of six slip systems leads to a strong work-hardening behavior due to slip system interaction processes.

Recent microcompression studies by Lilleodden [24] and Byer et al. [25] confirm that $\pi 2$ slip is the predominant deformation mechanism during *c*-axis compression of