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DEFORMATION BEHAVIOR OF MG FROM MICROMECHANICS TO ENGINEERING APPLICATIONS

E. Lilleodden, J. Mosler, M. Homayonifar, M. Nebebe, G. Kim, and N. Huber*
Institute of Materials Research, Materials Mechanics,
Helmholtz-Zentrum Geesthacht, Max-Planck-Str. 1, 21502 Geesthacht, Germany

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Abstract

We have investigated the influence of the underlying microstucture of Mg on its macroscopic deformation behavior. Using microcompression experiments on Mg single crystals, we have identified the orientation dependent deformation slip and twinning systems. These experiments have aided the development of an energy based crystal plasticity model for the twinning in polycrystals. This model has been applied to representative volume elements to identify the flow surface for a macroscopic model, which is used to predict the forming limit diagram. Validation of the results has been realized through Nakazima tests. Additionally an outlook is given on the prediction of the forming behavior of laser beam welded Mg sheets and its dependence on welding direction.

Introduction

Mg, the lightest of all structural metals, shows great promise for reducing weight in structural automotive applications, greatly improving fuel consumption and CO2 emissions. The development of new Mg alloys and joining technologies is an active area of research. In order to optimize alloy design and welding process parameters, the influence of alloying constituents and heterogeneity of microstructure on the mechanisms of deformation across the laser welded interface must be understood.

In order to develop a continuum model of such complex structural components, both a fundamental understanding of their constituent mechanical behavior at the microstructural level is needed, along with a continuum description of the mechanical behavior at the component level. While both ends of this broad spectrum necessitate in-depth investigations, the bridging of these scales is a critical challenge. In this paper, we present an overview of the scientific efforts across multiple length scales directed towards a comprehensive understanding of the mechanical behavior of Mg, with an outlook as to the applicability of such an approach to laser welded sheets.

Micromechanical characterization

Due to the potential involvement of both slip and twinning mechanisms during the deformation of Mg, the identification of the relevant deformation mechanisms under an arbitrary stress state cannot be known *a priori*. This is in strong contrast to face center cubic materials which show slip limited to the {111} planes. While the basal slip system is without debate the most easily activated system in Mg, it is less clear under what conditions prismatic slip and pyramidal slip systems are activated, or what the critical dependencies are for the activation of twinning. In order to identify slip and twinning activity in magnesium, the recently exploited method of microcompression testing [4,5] has been applied to single crystals of four model orientations: <0 0 0 1>, < 1 1 -2 0 >, < 1 0 -1 0 > and <2 -1 -1 2>. This same approach can be easily extended to studying the effect of alloying content and strain rate, which is the subject of a current investigation. The microcompression method is described elsewhere in detail [6].

Microcompression columns were fabricated from the bulk single crystals using focused ion beam machining, resulting in columns with a nominal diameter of 5μm and a height to diameter aspect ratio of approximately 3:1. Compression experiments were conducted with a Nanoindenter XP (Agilent) outfitted with a flat ended conical indenter with a 15 micron diameter circular punch. Experiments were run to varying maximum strain using a nominally constant strain rate of 0.001 /s. After compression, the columns were imaged in the SEM to assess the deformation morphology, such as slip steps. Cross sections were fabricated through columns with the FIB for conducting electron back-scattered diffraction (EBSD) analysis of orientation for the investigation of twinning. The FIB was also used to fabricate thin lamella for transmission electron microscopy (TEM) analyses of slip activity.

The engineering stress-strain curve of representative columns from each orientation is given in Figure 1. The associated deformed columns are shown in the SEM micrographs given in Figure 2. Unsurprisingly, the deformation behavior is strongly governed by the initial crystallographic orientation, as shown in the stress-strain response as well as the deformation morphology.

In the case of <0001> compression, relatively high stresses are achieved, with considerable hardening. Post-compression EBSD and TEM analyses have shown that no twinning occurs [6] and that pyramidal slip with a < c + a > Burgers vector is the dominant mechanism of deformation. The high hardening observed can be easily rationalized by the activation of 6 equivalent slip systems, as dictated by the symmetry of this orientation.

In the case of compression along the <2 -1 -1 2> axis, the so-called 45° orientation, basal slip is the governing deformation mechanism, as expected; a large slip band is observed along the 45° plane. It is important to note that the slip band occurs in the middle of the column, rather than at a stress concentration at the contact or base. The associated stress-strain response shows a large strain burst at about 25 MPa, the lowest stress of all orientations. Of course this is still a relatively high stress for Mg

* Corresponding author: norbert.huber@hzg.de

single crystal oriented for easy slip on the basal plane. This high stress is due to the widely observed size effect in microcompression testing, where the flow stress is shown to increase with decreasing diameter [4-8]. While the basis for size effects in microcompression testing has been attributed to various factors, such as the depletion of dislocation sources with decreasing size [7] or a size dependent dislocation source length [8], it is beyond the scope of this paper to investigate the basis of the observed size effect. While the presence of the size effect complicates the use of microcompression testing for the validation of continuum models, in the context of this paper the microcompression data are used to establish the relevant modes of deformation and relative stress-strain responses as a function of orientation; quantification of the resolved shear stresses is not our objective here.

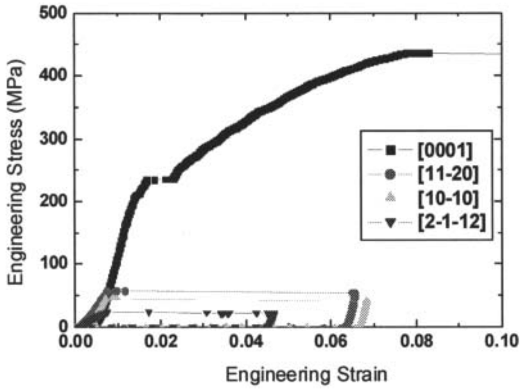

Fig. 1 Engineering stress-strain responses from respresentative columns of the 4 tested orientations, with nominal diameter of 5 μm.

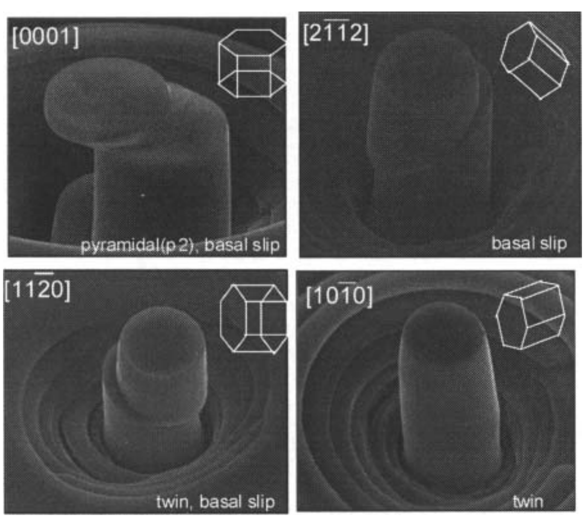

Fig. 2 SEM images of 5 μm diameter columns in Mg single crystals after compression.

The other two compression orientations: <11-20> and <10-10>, show intermediate stress levels relative to the <0001> and 45° orientations. Furthermore, they both show negligible hardening relative to the <0001> orientation, and a similar massive strain burst relative to the 45° orientation. However, deformation twinning is the primary mode of deformation for these two orientations, whereas no twinning was observed in the <0001> and 45° orientations. Compression along the <11-20> or <10-10> direction results in a tensile strain along the <c> axis which serves as the driving force for twinning. The massive strain burst shown for the <11-20> and <10-10> orientations has been shown to be due to a destabilization of the propagating twin [9], rather than a massive slip such as is observed in the 45° orientation. In case of <11-20> compression, the twin formed is well oriented for easy basal slip, which leads to massive shear on the basal system within the twin. This contributes to the strain burst observed in the stress-strain response in fig. 1, and typically leads to a larger burst than that observed in the <10-10> orientation. However, the strain burst is initiated prior to massive basal slip, as discussed in greater detail elsewhere [9].

Such a qualification of the deformation mechanisms in pure single crystal Mg as a function of orientation, as has been achieved here with microcompression testing, establishes which mechanisms are needed to be incorporated within a continuum framework. This can simplify both the development of a physically-based model, as well as allow higher efficiency in carrying it out. While at present, the values of critical resolved shear stresses for the individual slip and twinning mechanisms can not be obtained from the microcompression method, the relative stresses provide a starting point for a more accurate picture of deformation in Mg. The relevant slip and twinning systems identified from microcompression tests for a given stress state are used to develop a more physically based model of twinning. Ongoing work using dislocation dynamics simulations is being used to address the size effects in order to establish quantitative inputs for crystal plasticity modeling.

Micromechanical energy-based twinning model

While experimental characterization is an important element in understanding the mechanical behavior of materials, computational simulations are essential to the quantitative interpretation of results. This is particularly true for the aforementioned testing methods at the micron scale. For example, it is difficult if not impossible to observe the internal structure of a deforming body. Since the goal is the realistic prediction of mechanical behavior at the macro-scale, atomistic models are not promising. However, purely phenomenological macroscopic models are not suitable either, since the experimental observations cannot be directly included in this case. For this reason, the framework of crystal plasticity theory has been chosen. It naturally accounts for the different orientations of dislocations, but it is still numerically comparably efficient. In line with 0, twinning has been modeled as phase decomposition. For instance, highlighting the initial untwinned phase by the subscript (ini) and the twinned domain by (Tw), the total Helmholtz energy Ψ can be computed as the volume average, i.e.,

$$\Psi = (1 - \xi)\Psi_{\mathrm{ini}} + \xi\, \Psi_{\mathrm{Tw}} + \Psi^{\mathrm{mix}}(\xi). \qquad (1)$$

Here, $\xi \in [0;1]$ and Ψ^{mix} denote the relative twinning volume ratio and a mixture energy, respectively. Assuming that energy minimization is the underlying physical principle, the twinning volume ratio follows from minimizing Helmholtz (1). Since this function is highly non-linear and non-convex, its minimization cannot be computed in a straightforward manner. For this reason, only the limiting cases (completely untwinned or completely twinned crystal) have been considered. Since without additional modifications of the constitutive model, this would lead to a discontinuous stress response, the concept of twinning *pseudo dislocations* has been adopted, cf. [10]. Within this concept, the deformation associated with twinning is decomposed into a reorientation of the crystal lattice and a simple shear mode. The latter is modeled in an analogous fashion as dislocations.

The approach briefly discussed here can be generalized such that dissipative effects resulting from dislocations and twins are consistently included. Conceptually, the Helmholtz energy has to be replaced in this case by an incrementally defined potential denoted as I^{inc}. Further details are omitted. They can be found in [10]. The resulting optimization problem reads

$$I^{inc} = \min[I^{inc}_{ini}; I^{inc}_{Tw}]. \qquad (2)$$

This variational approach has been implemented into a finite element code. Subsequently, it has been applied to the analysis of texture evolution in a Mg polycrystal. The prescribed strain history corresponds to that of a rolling process. According to Fig. 3, the initial isotropic texture evolves and leads finally to a material with pronounced anisotropy. The computed results agree well with those previously reported in [11].

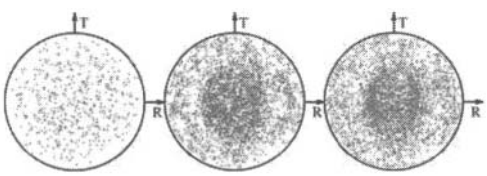

Fig. 3 Simulation of a rolling process by using the energy-based twinning model: Pole figure showing the evolution of the basal texture for different strain amplitudes. From left: ε = 0.00, ε = -0.68, ε = -1.20.

Macroscopic phenomenological plasticity model

Although the novel crystal plasticity model is computationally efficient and therefore can be used for the analysis of texture evolution in polycrystals, it is still numerically too complex for large scale engineering problems. For this reason, an additional model is introduced. It falls into the range of macroscopic finite strain plasticity theory. Its yield function was originally proposed in [12]. In tensor notation it can be rewritten as

$$\phi = J_2^{3/2}(\mathbb{H}_1 : \boldsymbol{\Sigma}) + J_3(\mathbb{H}_2 : \boldsymbol{\Sigma}) + h \leq 0. \qquad (3)$$

Here, J_2, J_3 are the second and the third invariant of the second order tensors $\mathbb{H}_i : \boldsymbol{\Sigma}$ and $\boldsymbol{\Sigma}$, is the stress tensor (of Mandel type), h denotes the current yield strength (isotropic hardening) and the fourth order tensors $\mathbb{H}_i$ define the material's anisotropy. In contrast to [12], they may evolve (distortional hardening) and thus, the shape of the yield surface may change during deformation, cf. [13]. Following computational homogenization techniques (see e.g. [14]), the material parameters of the macroscopic model briefly presented here are computed by considering representative volume elements (RVE) with periodic boundary conditions. More precisely, using the aforementioned novel crystal plasticity model within such RVEs allows the computation of macroscopic yield functions which can be subsequently used for calibrating the material parameters of the macroscopic model. For that purpose, a standard least-squares approach is used, i.e., the difference between the macroscopic yield function, which depends on the unknown material parameters, and the yield function computed from the RVE is minimized. Accordingly, these yield functions are associated with a rolled sheet showing a pronounced texture (see Fig. 3). The resulting model has been implemented into a finite element code. Results predicted by this model compared to experimental measurements on rolled sheets with thickness 1.3mm are shown in Fig. 4. Accordingly, the model captures the strain distribution in good agreement with the Nakazima forming limit test. This test has been re-computed for different sheets with different shapes. For defining the ultimate load, the localization criterion proposed in [15] was implemented. By way of contrast, the forming limit curve associated with the conducted experiments has been determined by synchronizing the ultimate load with the respective principal strains. The results are summarized in Fig. 5. As evident, the numerically computed forming limit diagram matches its experimentally obtained counterpart very well.

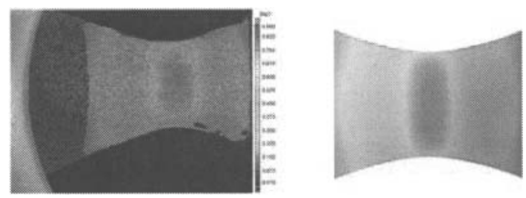

Fig. 4 Nakazima forming limit test for AZ31 with thickness 1.3 mm: contour plots of the maximum in-plane principal strain. Left: experiment; right: numerical results as predicted by the phenomenological macroscopic constitutive model, see Eq. (3).

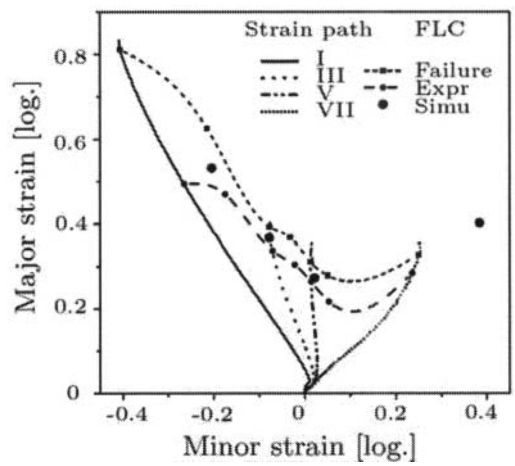

Fig. 5 Nakazima forming limit test for AZ31: comparison between experimentally measured forming limit curves and numerical simulations based on by the phenomenological macroscopic constitutive model, see Eq. (3).

Concluding remarks

We have shown that the deformation at the microstructural level can be integrated into a continuum framework for the simulation of sheet forming behavior of Mg alloys. The presented approach relies on the overlap between experiment and simulation at the micro-scale. Microcompression experiments provide the appropriate deformation mechanisms as constitutive inputs in crystal plasticity simulations. Through homogenization with representative volume elements the texture for a polycrystalline rolled material has been predicted. The resulting macroscopic yield functions, including their evolution, have been used to extend the existing macroscopic plasticity model of Cazacu and Barlat. Validation was achieved through experiment and simulation of Nakazima forming limit test for AZ31. The approach presented is currently being applied to laser-welded AZ31 sheets, a material system with a strong heterogeneity in microstructure and property distribution.

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