TOWARDS MICRO-MECHANICAL CHARACTERIZATION OF PLASTIC ANISOTROPY IN HEXAGONAL MATERIALS USING SHAPE MANIFOLD LEARNING

Mechanical characterization typically involves the use of a variety of mechanical tests such as uniaxial and biaxial tensile tests (for ductile materials such as metals and alloys), different compression tests (for brittle and quasi-brittle materials such as concrete) and relatively recent quasi-nondestructive tests such as instrumented indentation [1, 2], with the ultimate aim of determining its macroscopic mechanical plastic behavior: (e.g. yield surface, strain hardening, Lankford coefficients). Numerical simulation is widely adopted to complement, and in some cases replace, experimental tests and error methods in order to reduce the time and cost of development.

For several decades, material behavior has been described using phenomenological constitutive relations in the general framework of the theory of elasto-visco-plasticity. This approach, albeit useful for simulating boundary value problems in a realistic manner with the help of finite element methods, has potential limitations for very anisotropic materials. These could be improved upon by taking into account the fundamental mechanisms involved during mechanical deformation. Anisotropic behavior in hexagonal materials (Zn, Zr, Mg alloys) is often very difficult to properly characterize due to the effect of their microstructure and initial crystallographic texture. At the micro-scale level, metal plasticity involves the nucleation and migration of dislocations in the crystals and polycrystals as the underlying basis for microstructure evolution during plastic flow. As the individual crystals have different sizes and orientations, i.e., the crystallographic texture, the anisotropy of the mechanical properties of a polycrystal is a direct consequence of the anisotropy of the properties of each grain and of this crystallographic texture. Moreover, the reorientation of the grains during mechanical deformation of the polycrystal results in texture changes.

Hexagonal Close Packed (HCP) materials can be deformed by two different mechanisms: slip and twinning. Slip in the crystallographic planes is the principal mechanism, which is activated when the resolved shear stress reaches a critical value. This critical value is lower along close-packed planes due to the higher atomic density, and therefore slip along these

planes is the preferential way to accommodate plastic deformation. The second mechanism, twinning, is also activated particularly at higher loads, along several directions of the crystal, and with a separate critical stress value. Twinning leads to a discrete rotation of the c-axis within the twinned volume, by an angle depending on the type of the activated twin system. Several twin families have been identified in HCP materials: (1 0 -1 2), (1 0 -1 -3), (1 0 -1 1), (1 1 -2 -4), (1 1 -2 2), (1 1 -2 1), with the activated twin mode(s) depending on the c=a of the material. Surprisingly few studies, if any, are devoted to the mechanical characterization and to the study of the anisotropic behavior of this class of materials as a function of the initial microstructure, despite the continuing widespread use of these materials. In his seminal work on the ductility of polycrystalline metals [3], von Mises was the first to note that five independent slip systems were required to accommodate the strain requirements associated with an arbitrary homogenous plastic deformation. Metal plasticity would require a (nearly) traceless deformation rate tensor with only 5 independent components (i.e. unknowns), needing a system of 5 independent deformation mechanisms (equations). While this criterion is directly applicable to Face-Centered Cubic (FCC) and Body-Centered Cubic (BCC) materials, the fundamentals of the yielding and work hardening response for hexagonal metals are significantly more complex, mainly because the hexagonal lattice does not provide a sufficient number of geometrically equivalent slip systems to satisfy the Von Mises criterion for polycrystal deformation, which is very different from what is seen in the case of FCC and BCC lattices. Meanwhile, to accomplish the deformation, more than one crystallographic slip mode and/or twin mode must be activated. The exact deformation mechanisms in Hexagonal Close Packed (HCP) metals, dislocation motion on specific slip systems and activation of twinning, are not yet completely understood. This means that HCP materials show markedly anisotropic mechanical properties that depend on its initial textures, deformation mechanisms and critical shear stresses which, in turn, are different for different slip systems as well as the direction of the applied stress (e.g. asymmetry of twin activation) during mechanical loading. There are four possible slip systems, basal, prismatic and pyramidal < a > and pyramidal < c+a >. In general, zinc exhibits deformation on several crystallographic slip and twin systems, with very different activation stresses for each system. The relative contributions of individual slip and twin modes strongly depend on temperature, loading conditions, alloying elements, crystallographic texture, and microstructure evolution. This is the main reason for zinc's anisotropic behavior. The differing volume fractions of twins during tensile and compressive loading leads to the alloy's tension-compression asymmetry. Nevertheless it can be noticed that basal and pyramidal < c+a > are more likely

to be activated in the tensile test [4]. Furthermore, some alloys have an c/a considerably higher than that of an ideal structure (c/a = 1.632) and this leads to a higher than usual property dependence on the slip and twinning systems, e.g. Zinc alloys [5].

Currently, there is a dearth of systematic studies where crystallographic texture and grain anisotropy have been examined over a wide range of conditions. Knowledge of the active deformation mechanisms and the variation in their relative contribution as a function of these variables is required for accurately predicting the plastic response and texture evolution of this class of alloys. This is particularly important for the development of reliable material models for use in simulating forming processes with these materials, especially given the increase in applications of this class of materials.

The existing literature on mechanical modeling of the anisotropy of hexagonal materials is based on micro-mechanical approaches [6,7]. Micro-mechanical modeling provides a link between the microstructure of a material and its mechanical behavior, allowing us to quantify plastic deformation at the microstructural level. This approach is thus well-suited for simulations involving material texture and related anisotropy. A considerable amount of simulation has been performed using "physically based" models rather than simply fitting phenomenological behavior laws in the literature [6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16].

Some of these alloys typically involve both slip as well as twinning modes. These systems have different and unknown activation stresses that depend, usually in a non-unique manner, on the experimental approach used to study the texture as well as on the type of micro-mechanical model. We therefore need an accurate model to simulate its deformation under loading, including the large deformations typically encountered during forming processes. This model needs to be capable of not just describing the mechanical response of the material for a given texture, but also predicting how this texture would evolve with deformation.

Due to their significant anisotropy, the experimental forming set up which allows the realization of the desired complex shapes is time consuming and judicious sequences of several forming steps should be achieved in order to reach the desired forms. The optimization of such sequences can be readily accomplished based on numerical simulation using more phenomenological and physical models suitable for these materials. In the recent years much less attention has been dedicated to the experimental characterization and the macroscopic modeling of the anisotropic behavior of this class of alloys under several loading paths at finite strains in spite of the continuing widespread use of these materials.

Cauvin et al [17] presented a complete protocol for the characterization of hexagonal polycrystalline alloys by clarifying the physical mechanisms involved in the plastic

deformation of rolled Zn-Cu-Ti sheets, using only tensile testing along three directions and Electron Beam Scatter Diffraction (EBSD) to examine the microstructure i.e. texture evolution. The Visco-Plastic Self-Consistent (VPSC) model is considered to estimate the multiscale behavior of the rolled Zn-Cu-Ti sheet, with the required material parameters such as the critical resolved shear stresses for the different slip and twin systems identified using an inverse analysis by comparing the stress-strain curves from uniaxial tensile testing along three different orientations (0_/RD, 45_/RD and 90_/RD) along with the simulated macroscopic stress-strain curves along the same three directions. The inverse problem is solved by optimization with the well-known Covariance Matrix Adaptation Evolution Strategy (CMA-ES) [18] evolutionary algorithm.

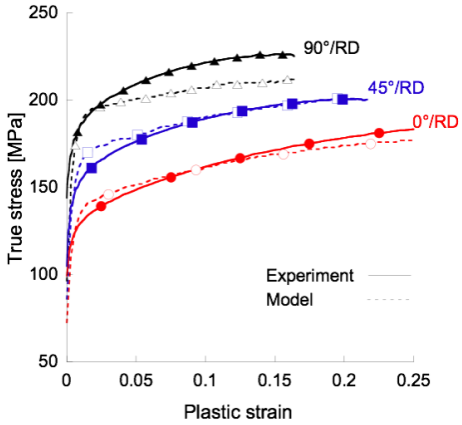

Figure 1: Tensile test: simulations vs. experimental data [17].

As shown in the figure 1, with the identified parameters, a good agreement between the simulation and the experimental data is obtained for the 3 considered directions. Using the identified micro-scale parameters, we calculate the Lankford R-values followed by the Hill coefficients for the alloy by simulation (Fig. 2). The simulated and experimental yield surfaces are compared (Fig. 2).

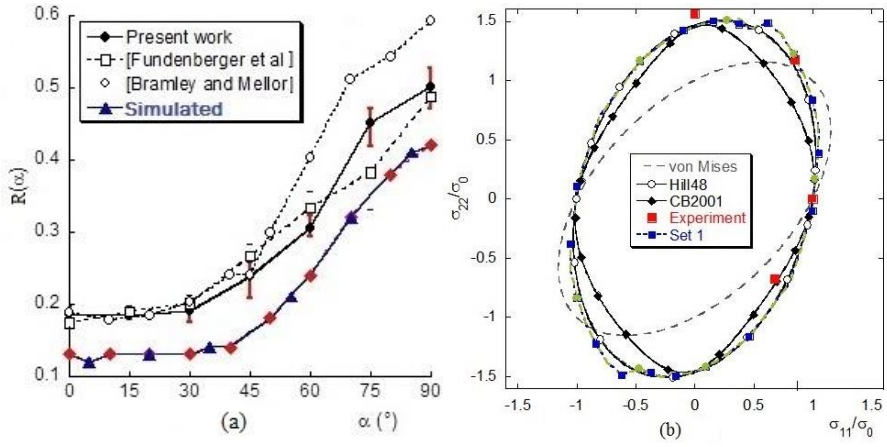

Figure 2: Comparison between experimental data and simulations [17]: (a) Lankford coefficients (b)Yield surface

Finally, the simulated R-values are compared with those reported in the literature [19, 20] (Fig. 2). However, the multi-scale computational approach had two main shortcomings:

1. Like all micro-mechanical modeling approaches, the amount of computational effort and time were exorbitant.

2. The pole figures were only used to appraise the quality of the identified parameter sets and not directly used in the inverse problem.

This leads to a need for reduced-order modeling techniques to attempt to correct both shortcomings at the same time, which could potentially be achieved in short order using the shape manifold approach to both reduce the number of computations as well as to reduce computation time per calculation (parameter set).

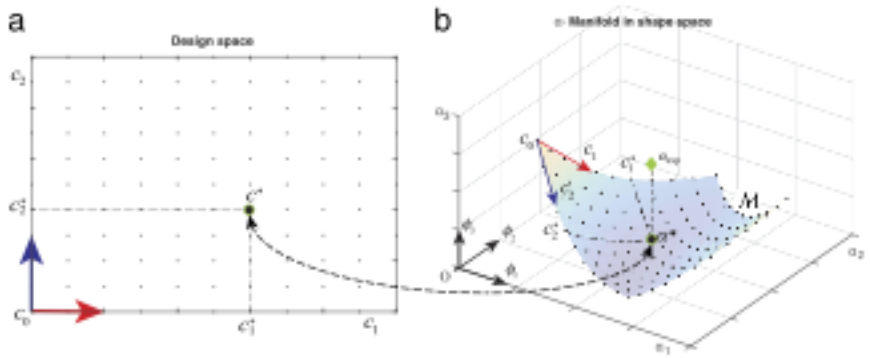

Figure 2: Notion of shape space for the pole figures

The idea is to (eventually) develop a shape manifold-based approach capable of "learning" the anisotropy intrinsically "encoded" in the pole figures, allowing for a direct comparison of the simulated and experimental mesostructures, to identify the micro-mechanical parameters and eventually the macroscopic properties.

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