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On the strength of dislocation interactions and their effect on latent hardening in pure Magnesium

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ABSTRACT

This study is dedicated to the quantification of latent hardening and its effect on the plasticity of pure hexagonal magnesium. To this end, discrete dislocation dynamics simulations are used to (1) extract latent hardening parameters coupling different slip systems, and to (2) assess the validity of two existing constitutive models linking slip system strength to dislocation densities on all slip systems. As hexagonal materials deform via activation of different slip modes, each with different mobilities and lattice friction stress, the effects of the latter on latent hardening evolution are also investigated. It is found that the multi-slip formulation proposed by Franciosi and Zaoui gives accurate predictions when multiple interactions are involved while the formulation suggested by Lavrentev and Pokhil systematically overestimates the flow stress. Similar to FCC materials, it is also found that collinear interactions potentially contribute the most to latent hardening. Basal/pyramidal $\langle c+a \rangle$ interactions are found to be very strong, while interactions involving second-order pyramidal $\langle c+a \rangle$ primary dislocations appear to be the weakest ones. Finally, the latent hardening parameters, extracted from the discrete dislocation dynamics simulations, are used in polycrystal simulations and the impact of finely accounting for latent hardening on predictions of the macroscopic anisotropic response is shown to be of significant importance.

1. Introduction

In crystalline media, strain hardening primarily results from interactions of material defects, such as dislocation–dislocation, twin–dislocation and twin–twin interactions. While the two last contributions remain a very important issue and are actively studied, especially in the case of hexagonal close-packed (HCP) (e.g. Capolungo et al. (2009) and Yu et al. (2013)), this study is dedicated to dislocation–dislocation interactions. Early on, it has been established that, in addition to the lattice friction stress, the flow stress is proportional to the square root of the dislocation density (Taylor law) during plastic deformation of metals (Kocks and Mecking, 2003). This law can be directly related to the mean free path of dislocations, i.e., the mean spacing between forest dislocations acting as obstacles for a moving dislocation (Basinski, 1959; Cottrell, 1953; Foreman and Makin, 1966; Kuhlmann-Wilsdorf, 1962; Saada, 1960). While early models solely relied on the total dislocation density, Franciosi and Zaoui (1982) and Lavrentev and Pokhil (1975b) have proposed different extensions of the Taylor-law

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accounting for individual slip systems dislocation densities, introducing latent-hardening interaction coefficients pertaining to the strength of the different dislocation–dislocation interactions between slip systems. Latent-hardening matrix parameters have become a key ingredient in dislocation density-based crystal plasticity models (Devincre et al., 2006; Kubin et al., 2008). Their accurate evaluation was found to be important for modeling and predicting the mechanical response of materials. For example, Hoc et al. (2004) found that the orientation dependence of stage I deformation of face-centered cubic (FCC) crystals was strongly linked to the values of the hardening coefficients, and the relatively large values associated with collinear interactions have explained the unique selection of slip activation in orthogonal loading (Devincre et al., 2006; Madec et al., 2003). Also, for complex loadings paths, such as strain path change, latent hardening is expected to play an important role in material response (Gerard et al., 2013; Rauch et al., 2011). However, current constitutive models developed for HCP materials incorporate latent hardening models that are not directly related to the microstructure, but whose parameters are obtained by a fitting procedure. For example, slip induced hardening is described through a Voce law (Proust et al., 2007; Wang et al., 2013) or using a single hardening coefficient in a dislocation density law (Beyerlein and Tomé, 2008; Knezevic et al., 2013; Oppedal et al., 2012).

Several efforts have been dedicated to evaluate these coefficients. Analytical approaches were used by Lavrentev and Pokhil (1975b) and Lavrentev (1980), where values of the coefficients were assumed to be related to the energy gain due to pairwise interactions of dislocations. Also, coefficients for different types of interactions were experimentally determined for Mg (Lavrentev and Pokhil, 1975a,b) at different deformation stages via latent hardening tests designed to introduce different forest densities on different slip modes. However, difficulties in measuring dislocation densities are likely to induce large uncertainty in experimental estimates for these coefficients.

As another means, discrete dislocation dynamics (DDD) simulations have allowed for a numerical quantification of the hardening coefficients. Madec (2001), Madec et al. (2003) and Devincre et al. (2006) have computed the coefficients for face-centered cubic metals and were able to construct junction formation maps for the nature of interactions as a function of the relative angle of the intersecting dislocation segments. In doing so, they also revealed the strong effect of collinear interactions in hardening (Madec et al., 2003). Using the same approach, Queyreau et al. (2009) computed the coefficients for BCC α-iron. In Monnet and Devincre (2006) and Queyreau et al. (2009), the effect of lattice friction was also investigated.

Compared to cubic crystals, considerably less DDD studies have been dedicated to the more complex case of HCP metals. Atomistic simulations have revealed 3D spread of prismatic dislocations cores (Bacon and Vitek, 2002) as well as strong anisotropies in dislocation mobilities and friction stress of slip systems (Groh et al., 2009). Such anisotropies in core properties were supported by in situ TEM experiments in which the presence of long screw segments – suggesting significant lattice friction and low mobility of such dislocations – was observed for prismatic dislocations (Caillard and Couret, 2002). In a first attempt to mimic such anisotropic properties, Monnet et al. (2004) used the DDD method where dislocation mobilities were modeled in a phenomenological manner to study prismatic slip in Zirconium. As a result, it was found that junctions could not be formed between screw dislocations. Using DDD as well, Capolungo (2011) investigated the strength of junctions in Mg relying on elastic interactions only. Similar work was further extended to Mg and Be (Wu et al., 2013). In such works, the formation and destruction of a single binary junction is studied, leaving collective effects and other possible interactions pertaining to latent hardening aside. Capolungo et al. (2010) also used DDD to show the weak effect of anisotropic calculations in the case of Mg, suggesting that an isotropic calculation could be safely used as an approximation. Nevertheless, to the authors' knowledge, except for ice single crystal (Devincre, 2013), hardening coefficients have not been calculated for hexagonal materials.

In addition, although the flow stress dependence on dislocation density has been verified against experimental data, the validity of multi-slip extensions, such as the ones proposed by Franciosi and Zaoui (1982), FZ, and Lavrentev and Pokhil (1975b), LP, has rarely been tested. To the authors' knowledge, Queyreau et al. (2009) were the only ones to verify the validity of the Franciosi and Zaoui formulation using DDD simulations on multi-slip conditions for BCC α-iron crystals, but the validity of the superposition principle expressed through these laws has never been discussed for HCP materials and the two multi-slip formulations have never been directly compared.

The goals of this work are to (1) quantify latent hardening coefficients based on both the FZ and LP models, (2) identify which model is more appropriate for HCP metals, and (3) assess the importance of finely accounting for latent hardening on the mechanical response of pure magnesium. The paper is organized as follows: Section 2 presents the different types of interactions that can occur in Mg during deformation. In Section 3, the methodology for computing the hardening coefficients for single crystal Mg is presented while the validity of the additive rule used in constitutive models is examined in Section 4. The effects of friction and mobilities are discussed in Section 5. Finally, the influence of the hardening coefficients on the macroscopic mechanical response of polycrystals is studied in Section 6 using the VPSC formalism.

2. Dislocation interaction types and latent hardening

2.1. Current approach in modeling latent hardening via constitutive approaches

In constitutive laws, the effects of dislocation interactions on the critical resolved shear stress (CRSS) are usually accounted for via an extended Taylor's law, which relates the CRSS on a given system to the total dislocation densities on