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A continuum model for initiation and evolution of deformation twinning

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ABSTRACT

Within continuum dislocation theory the plastic deformation of a single crystal with one active slip system under plane-strain constrained shear is investigated. By introducing a twinning shear into the energy of the crystal, we show that in a certain range of straining the formation of deformation twins becomes energetically preferable. An energetic threshold for the onset of twinning is determined. A rough analysis qualitatively describes not only the evolving volume fractions of twins but also their number during straining. Finally, we analyze the evolution of deformation twins and of the dislocation network at non-zero dissipation. We present the corresponding stress–strain hysteresis, the evolution of the plastic distortion, the twin volume fractions and the dislocation densities.

1. Introduction

The characteristics of plastic deformation of engineering materials depend to a high degree on the material microstructure comprising all structural characteristics on the microscale, which range from one-dimensional point defects such as vacancies or solute interstitials to the two- and three-dimensional lattice defects such as dislocations, grain and phase boundaries, or particulate inclusions, to mention only a few. Along with the properties of the periodic crystal lattice, all of these microstructural defects are integral components to determine the macroscopic mechanical response of the material. The most important mechanism for plastic flow is the nucleation and interaction of the dislocation network within the crystal lattice. Dislocation sliding and climbing accommodate plastic deformation, cross-slip or pinning of dislocation are only two examples of mechanisms responsible for hardening by plastic slip. Furthermore, dislocations are not only a key microstructural defect for plastic slip but also the core ingredient for forming microstructural patterns and substructures. The formation of microstructural patterns has been observed experimentally and has been subject to intensive investigation, based on the early works by Ericksen (1975) and Ball and James (1987), and followed by a variety of novel approaches in recent years, see e.g. Govindjee et al. (2003), Carstensen et al. (2002), and Ortiz et al. (2000).

Besides plastic slip of dislocations, there is another important mode of plastic deformation in many crystalline solids, known as deformation twinning. Slip and twinning are the major deformation modes which accommodate a change of shape under the action of applied tractions or displacements. Experimental evidence for deformation twinning was found long time ago and described in terms of dislocations e.g. in the early works by Frenkel and Kontorova (1939), Cahn (1954), and Hall (1954). A newer comprehensive state-of-the-art survey of deformation twinning from a rather materials science perspective was presented by Christian and Mahajan (1995). A recent very comprehensive experimental study of the

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competing mechanisms of slip and twin in Zr and Mg alloys was presented in a series of papers by Kaschner et al. (2006, 2007) and Proust et al. (2009). Deformation twins have been reported to occur especially in b.c.c., h.c.p. and lower symmetry metals and alloys but also in many f.c.c. metals and alloys with low stacking-fault energy, or other intermetallic compounds as well as in geological materials such as calcite or quartz. Twinning becomes particularly important in metals with only a limited number of slip systems, as it can operate to provide the five slip systems required to satisfy the criterion for a general slip deformation. Deformation twinning basically divides the originally uniform single crystal into two volumetric parts—a parent phase (with unaltered crystal lattice) and a twin phase (with a different crystal lattice orientation). Both phases normally occur in the form of lamellar structures, where a bicrystal consisting of neighboring parent and twin phase is commonly referred to as a *twin*. The twin lattice can be generated either by a rotation of the original crystal lattice by 180° about some axis (mode I) or by reflection in some plane (mode II) so that in both cases—when joint with the undistorted parent phase—an unfaulted single crystal is formed, which exhibits a twin boundary with coincident lattice positions at the interface. This topic is closely related to martensitic phase transformations and the observed effect of transformation induced plasticity (TRIP). In this paper, however, we will limit our analysis to the effects of twinning induced plasticity (TWIP).

The formation of deformation twins has significant impact on the macroscopic stress–strain response. The evolution of twins provides TWIP alloys with excellent hardening behavior (Allain et al., 2004), allowing for higher stresses and larger strains than in common f.c.c. or b.c.c. metals. As a special characteristic, the onset of twinning, i.e. the rapid nucleation of deformation twins, often gives rise to a large load drop in the stress–strain behavior (Christian and Mahajan, 1995). The increase of strength and work hardening during microstructure refinement by twinning in manganese steels or other TWIP-alloys remains until now not quite well understood. Perhaps the dislocation pile-up near the twin boundaries (raising the boundary energy) and the related size-effects play an important role here. Experiments on single crystals have shown that particularly f.c.c. metals normally do not twin before appreciable plastic deformation by dislocation slip has occurred, while e.g. b.c.c. metals often exhibit deformation twinning even in the elastic region before the onset of macroscopic yielding. It is, however, well accepted that twinning in metals is often accompanied or preceded by microslip and that the formation of deformation twins is initiated by pre-existing dislocation configurations which dissociate into twin boundary structures. Furthermore, it is believed that the finite boundary energies accompanying the pile-up of dislocations limit the refinement of microstructure and hence are responsible for the formation of discrete twin patterns. Since the earliest evidence of twinning, several efforts have been undertaken to incorporate twinning in material modeling to predict the stress–strain behavior. Several dislocation-based mechanisms have been proposed (Cohen and Weertman, 1963; Venables, 1964; Hirth, 1964; Narita and Takamura, 1992) to explain twin nucleation in f.c.c. materials. Most of these models are based on phenomenological observations rather than physically reasoned on the microscale.

In this paper, we present a micromechanical model to describe the initiation and evolution of deformation twins in metals and alloys by employing a continuum dislocation approach. This approach is dictated by the high dislocation densities accompanying plastic deformations, which are in the range of 10^8–$10^{15}\,\mathrm{m}^{-2}$, as well as the complexity of the dislocation network. Although the fundamentals of continuum dislocation theory were laid down long time ago by Kondo (1952), Nye (1953), Bilby et al. (1955), Kröner (1958), Berdichevsky and Sedov (1967), and Le and Stumpf (1996a, b), the applicability of the theory became feasible only in recent years (Ortiz and Repetto, 1999; Ortiz et al., 2000; Berdichevsky, 2006b; Groma et al., 2007) thanks to the progress in statistical mechanics and thermodynamics of the dislocation network (Le and Berdichevsky, 2001; Berdichevsky, 2005, 2006a; Hochrainer and Zaiser, 2005). Among various dislocation-based plasticity theories we mention here only those of Gao et al. (1999), Acharya and Bassani (2001), Huang et al. (2000, 2004), Fleck and Hutchinson (2001), Han et al. (2005a, b), Aifantis and Willis (2005), Aifantis et al. (2006), which are closely relevant to our approach. Most of these works make use of the concept of geometrically necessary dislocations (GND) based on Nye's (1953) tensorial description, later propagated by Ashby's (1970) seminal paper. All of these strain gradient plasticity theories have as a common feature the incorporation of higher order strain gradients into the formulation of the free energy, thus taking into account the energy of the dislocation network. In this paper, we adopt the logarithmic formulation proposed by Berdichevsky (2006b) for the dependency of the energy of the dislocation network on Nye's dislocation density.

Based on this energetic approach, Berdichevsky and Le (2007) found the analytical solution of an anti-plane constrained shear problem for single crystals. Interesting features of their solution are the energetic and dissipative yielding thresholds, the Bauschinger translational work hardening and a size effect. The dislocation nucleation admits a clear characterization by the variational principle for the final plastic states (Berdichevsky, 2006b). Le and Sembiring (2008a) obtained the solution of the plane-strain constrained shear of a single crystal strip which exhibits the same features as that in Berdichevsky and Le (2007). Comparison with the results of discrete dislocation simulations obtained by Needleman and Van der Giessen (2001) and Shu et al. (2001) shows good agreement between the discrete and the present continuum approach (Le and Sembiring, 2008a). As a first step towards modeling deformation twinning, Kochmann and Le (2008a, b) studied the dislocation pile-up near the boundaries of a bicrystal. The solution exhibits similar characteristics as for the single crystal.

A new ingredient of this theory compared with our previous studies (Kochmann and Le, 2008a, b) is the so-called twinning shear produced by the existing dislocations in the already active slip system, which plays a similar role as Bain's strain in the theory of martensitic phase transformations, see e.g. Bhattacharya (2003). This twinning shear followed by a rotation enables the initially homogeneous crystal to form the twin phase from the parent phase. The underlying