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Thermostatistical modelling of hot deformation in FCC metals

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ABSTRACT

A novel thermostatistical approach to describe hot deformation of unary and multicomponent FCC alloys undergoing dynamic recrystallization (DRX) is presented. The approach incorporates an additional softening effect to the Kocks–Mecking equation, which becomes active once a critical incubation strain for recrystallization is achieved. Multicomponent effects are incorporated into the equation to account for solid solution strengthening and recrystallization effects. The dislocation density evolution with strain can be prescribed as a function of temperature, strain rate and composition. The presented unified approach describes stages II, III and IV of deformation, the latter being substituted by DRX when this becomes energetically favourable. It recovers the stress values as steady state is approached, and captures well the temperature-strain rate-composition dependency of DRX allowing to map the conditions under which it occurs. The theory successfully describes the dynamic recrystallization behaviour of Cu, Ni, Ni30Fe, Ni21Cr, Fe30Ni, Fe18Cr8Ni, Fe25Cr20Ni and Ni21Cr8Mo3Nb. Input to the model are only physical parameters and thermodynamic information from well accepted databases. It is shown that the design of alloys for tailored DRX behaviour is possible under this formulation.

1. Introduction

Predicting the conditions for the occurrence of dynamic recrystallization (DRX) during hot deformation of metals remains a problem of great technological importance as their mechanical properties become severely changed. Many efforts have been proposed to describe DRX. Lee et al. (2010) combined a cellular automata model to predict grain coarsening and refinement with the Kocks–Mecking equation describing the dislocation evolution in pure copper. Okuda and Rollet (2005) have employed Monte Carlo simulation methods to investigate the grain growth behaviour (misorientation and mobility) of a grain nucleus when particle pinning takes place in steels. Takaki et al. (2008, 2009) have modelled dynamic recrystallization with a multi phase field modelling approach, defining each growing grain as a phase field; the dislocation evolution is obtained by employing the Kocks–Mecking equation and it is combined with the phase-field simulation to estimate the recrystallization effect. Brown and Bammann (2012) combined a deformation gradient method with thermodynamics to describe the evolution of static and dynamic recrystallization in oxygen-free high conductivity (OFHC) copper; once again, a Kocks–Mecking-type equation is introduced to describe the dislocation evolution in the material, and an empirical function of the recrystallization volume fraction and the interfacial area between recrystallized and unrecrystallizaed grains is introduced; this relation is combined with an expression for grain boundary mobility to obtain the recrystallization fraction evolution; these equations are solved together to obtain the flow stress response. Fan and Yang (2011) have proposed an internal-state-variable model to describe dynamic recrystallization in a two-phase titanium alloy; the description of the

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dislocation density is given by the Kocks–Mecking equation, where the annihilation coefficient is expressed in the form of an Arrhenius equation (similar to what the authors have obtained (Galindo-Nava et al., 2012)). An additional term is introduced into the equation to account for dynamic recrystallization softening; this term is null until a critical (incubation) strain is reached, and is function of the grain boundary velocity and the grain boundary area per unit volume; an evolution equation is proposed for the latter including the contributions of grain nucleation, growth and impingement. Additional secondary phase effects are also considered in the constitutive equations. On the other hand, Cram et al. (2009, 2012) have postulated a polycrystal mean-field model where the evolution of each grain is described and embedded into an average medium, a Rayleigh probability distribution describes the subgrain size patterning, where a critical size for grain nucleation is taken as the condition for grain nucleation; grain growth evolution is postulated to be proportional to the grain boundary mobility and the difference between the total dislocation density and the dislocation density of the growing grain; the total dislocation density equals the surface-area-weighted dislocation average over all grains. The macroscopic stress is equated to the volume average of the stress over all grains.

Although these methods provide a description of DRX, phenomenological or empirical relations between the internal microstructure evolution and deformation conditions are introduced, and a number of parameters are fitted for each material, impeding their extension to more complex systems. Moreover, it has not been possible to produce a unified approach able to describe plasticity at different scales for deformation conditions when dynamic recovery and/or dynamic recrystallization are present (McDowell, 2010).

One of the most employed phenomenological models to describe dislocation behaviour is the Kocks–Mecking (KM) formulation, which accounts for the competition between dislocation generation and annihilation, describing the evolution of the average dislocation density ρ during deformation (Kocks and Mecking, 2003). This approach is directly applied to obtain the flow stress during deformation or it is incorporated into more complex techniques such as crystal plasticity, micromechanics or discrete dislocation dynamics, providing the material's hardening behaviour via the average dislocation density (Benkaseem et al., 2007; Favier and Barbier, 2012), the microstructural development on different slip systems (Lee et al., 2010; Alcalá et al., 2008; Keller et al., 2012; Liu et al., 2011), and the temperature and strain rate effects on plasticity (Beyerlein and Tomé, 2008; Oppedal et al., 2012). Examples of the use of KM approach as input to other modelling techniques to describe various deformation phenomena are shown in Table 1. Furthermore, as discussed above, several approaches describing dynamic recrystallization have employed this equation.

A recent approach has been postulated to describe plastic deformation of FCC pure metals across the scales (single crystals, coarse-grained polycrystals, dislocation cells and nanotwinned structures) at a variety of strain rates, and from cryogenic to high temperatures (Galindo-Nava et al., 2012; Galindo-Nava and Rivera-Díaz-del-Castillo, 2012d; Galindo-Nava and Rivera-Díaz-del-Castillo, 2012c; Galindo-Nava and Rivera-Díaz-del-Castillo, 2012a). Such formulation is based on finding an expression for the dynamic recovery rate f_{DRV} in terms of physical parameters; it employs a thermostatistical analysis on a dislocation segment undergoing annihilation without the introduction of artificial parameters. This term is incorporated into the Kocks–Mecking equation. The approach has also succeeded in prescribing the conditions for the formation of dislocation cells and their average size (d_c), as well as the occurrence of stage IV of deformation (Galindo-Nava and Rivera-Díaz-del-Castillo, 2012c).

The objective of the present work is to extend the previous approach for describing the conditions for dynamic recrystallization, and its evolution in FCC single phase alloys. At high temperatures and/or low strain rates, dislocation-free grains nucleate and grow from highly dislocated subgrains, decreasing the total dislocation density (Humphreys and Hatherly, 2004). The dislocation annihilation rate due to dynamic recrystallization is proportional to the dislocation density inside the growing grains that overtake the deformed zones. As deformation continues, the dislocation density inside the growing

Table 1
Modelling approaches employing Kocks–Mecking (KM) formulation as input: crystal plasticity (CP), finite element modelling (FEM), micromechanics (MM), discrete dislocation dynamics (DDD), Mesoscale/internal-state-variable (ISV).

Modelling technique	Physical Phenomena	Reference
CP/FEM	Deformation in single crystals	(Lee et al., 2010)
CP/FEM	Pyramidal indentation in FCC metals	(Alcalá et al., 2008)
CP/FEM	Softening kinetics in polycrystalline nickel with different sample thicknesses and grain sizes	(Keller et al., 2012)
MM	Twinning-induced plasticity in steels	(Favier and Barbier, 2012)
MM	Multiscale modelling of nanocrystalline materials	(Benkaseem et al., 2007)
DDD	Thin-film plasticity	(Liu et al., 2011)
ISV	Temperature effects of twinning in zirconium	(Beyerlein and Tomé, 2008)
ISV	Twinning hardening in magnesium	(Oppedal et al., 2012)