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Modelling multiscale plasticity: A thermostatistical approach

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Plastic deformation in single crystals, coarse-grained polycrystals, micrometric dislocation cells and nanotwinned structures are all described with a single formulation. The statistical entropy associated with the dislocation paths available for slip and twinning features strongly in the solution, allowing for the description of stress–strain relationships as a function of strain and strain rate, for very wide temperature ranges. The model is applied to determine the characteristic plastic behaviour across the scales for pure copper.

Keywords: Thermodynamics; Modelling; Statistical thermodynamics; Dislocation theory; Nanostructure

A frequently employed model to describe plastic deformation is the Kocks–Mecking formulation [2], wherein the average dislocation density ρ is the main parameter that evolves throughout deformation, and incorporates dislocation storage and annihilation terms. In general, the parameters employed in multiscale approaches are obtained by fitting them to experimental data to describe the behaviour of specific systems. This becomes difficult to predict or design for new properties as the parameters change with composition and microstructure.

In a recent review, McDowell [3] stated that "thermodynamics and kinetics relations are at the core of evolution equations for microstructure". The present work is an attempt to wrap together transitions at various scales by supplying a thermostatistical foundation to the Kocks–Mecking formulation across the scales under a variety of deformation conditions. Copper is taken as the model material, and the theory has been able to describe single crystal deformation behaviour; the formation, size and misorientation of micrometre-scale dislocation cellular structures; as well as the characteristic stress–strain response of nanotwinned and coarse-grained microstructures.

A key feature of this theory is the introduction of the statistical entropy ΔS that incorporates the possible paths for dislocation motion. Other than quantifying the slip systems that are likely to become activated, the paths that are energetically *favourable* at a given temperature and strain rate are considered. A microstate is defined as the number of interatomic subunits a dislocation segment glides during an arbitrary time step [4]. At high temperatures, where vacancy-assisted dislocation climb prevails, additional microstates are incorporated to account for their interaction [5]. The total number of microstates Ω_{int} becomes [4,5]:

$$\Omega_{int} = (\Omega_{dis} + \Omega_{v-d})^{\mathcal{N}} = \left(\frac{\dot{\varepsilon}_0}{\dot{\varepsilon}} + \frac{\vartheta}{\dot{\varepsilon}}\right)^{\mathcal{N}}, \tag{1}$$

where Ω_{dis} and Ω_{v-d} are the number of microstates due to dislocation slip and to vacancy–dislocation interactions, respectively; $\dot{\varepsilon}$ is the axial strain rate; $\mathcal{N}$ is the impingement effect due to the overlapping strain field of contiguous dislocations that alter the possibilities for dislocation slip, and is related to the stacking fault energy of the material[1]; $\dot{\varepsilon}_0 = cb\rho_Y$ is the limiting value for the strain rate, a constant related to the speed of sound in the material (c); b is the magnitude of the Burgers vector; $\rho_Y = (\sigma_Y/\alpha M\mu b)^2$ is the dislocation density consistent with the yield point, where $\alpha = 0.3$ is a thermal constant [2], $M = 3$ is the Taylor factor [2] and μ is the shear modulus; and $\vartheta = \vartheta_D \exp\left(-\frac{E_m}{RT}\right)$ is the vacancy migration frequency, wherein $\vartheta_D = 10^{13}\ \mathrm{s}^{-1}$ is the Debye frequency and E_m is the vacancy migration

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[1] Refer to [4] for the calculation procedure of $\mathcal{N}$.

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energy. The statistical entropy incorporating the dislocation's kinetic effect then becomes [4,5]:

$$\Delta S = k_B \ln \Omega_{int} = k_B \ln \left(\frac{\dot{\varepsilon}_0 + \vartheta}{\dot{\varepsilon}} \right)^{\mathcal{N}}. \tag{2}$$

The dislocation density evolution is obtained by reformulating the Kocks–Mecking approach and expressing the dynamic recovery coefficient (f) in terms of physical parameters within the thermostatistical framework [4,2]. An additional term (C) accounting for dislocation storage if nanotwins are present, thereby impeding the dislocation's motion, is incorporated [6,7]:

$$\frac{d\rho}{d\gamma} = \underbrace{\frac{k_1}{b}\sqrt{\rho}}_{(A)} - \underbrace{f\rho}_{(B)} + \underbrace{\frac{N_{nT}}{bD_{TB}}}_{(C)}, \tag{3}$$

where $k_1 = \frac{1}{30}\left(\frac{\mu}{\mu_0}\right)^2$ is the dislocation storage coefficient [2], μ_0 is the shear modulus at 0 K, D_{TB} is the average nanotwin-boundary thickness and N_{nT} is the dislocation storage term due to the presence of nanotwins. Note that, when coarse-grained polycrystalline metals are analysed, the term (C) vanishes as $D_{TB} \to \infty$. f is equal to [4,5]:

$$f = \frac{N_A \rho_a b^2 l^*}{w_a} \frac{\mathcal{N} T \Delta S}{\frac{1}{2}\mu b^3 + \sigma_Y A_{act} b^3 + \frac{l^*}{b}\delta(T)(E_f + k_B T \ln c_m) - \mathcal{N} k_B T \ln\left(\frac{\dot{\varepsilon}_0 + \vartheta}{\dot{\varepsilon}}\right)}, \tag{4}$$

where N_A is Avogadro's number; w_a is the material's atomic weight; ρ_a is the material's density; l^* is the dislocation's distortion field length (~98% of the total strain field induced by the dislocation [4]); $A_{act}b^2$ is the activation area for cross-slip[2]; E_f is the vacancy formation energy; c_m is the vacancy concentration at the melting point (T_m); and $\delta(T)$ is a continuum piecewise function [5], due to which the vacancy contribution vanishes ($\delta = 0$) at low temperatures ($T < T_0$), where $T_0 = \frac{E_m}{R \ln(\vartheta_D/\dot{\varepsilon})}$, below this value, the governing annihilation process is slip/cross-slip [2]; $\delta(T)$ becomes fully present ($\delta = 1$) at high temperatures ($T > T_f$), where vacancy-assisted dislocation climb prevails [8], where $T_f = \frac{E_m}{R \ln(\vartheta_D/\dot{\varepsilon}_0)}$. In the regime $T_0 < T < T_f$, $\delta(T)$ incorporates a mixture of cross-slip and vacancy-assisted climb processes [5].

The shear stress τ is obtained from the Taylor relation [2] $\tau = \alpha\mu b\sqrt{\rho} + \tau_D$ [2], where τ_D is the shear back stress induced when nanotwinning is present, impeding the motion of other dislocations [9]. It is worth noting that τ_D is neglected for single crystal/polycrystalline materials.

At the micrometre scale, dislocation cellular structures are formed on deformation. Although their average size is known to scale with $\rho^{-1/2}$ [10], the proportionality constant is usually fitted to experiments, as it varies with temperature and strain rate. The changes in the average cell size (d_c) can be obtained by performing an energy balance between the energy stored in the dislocation cell in the form of partials and the addition of the energy of the dislocation forest in the non-cellular material plus the dislocation slip energy to form the cellular structures; the latter is approximated by the statistical entropy for dislocation motion [11]. The resulting relation becomes: $d_c = \frac{\kappa_c}{\sqrt{\rho}}$, where $\kappa_c = \frac{12\pi(1-v)}{(2+v)}\left(1 + \frac{\mathcal{N}^{-1}T\Delta S}{\frac{1}{2}\mu b^3}\right)$ [11] and $v = 0.33$ is the Poisson ratio [12]. It is important to note that no additional parameters are incorporated in this formulation.

Another property of dislocation cells that is of great relevance for technological applications at the submicrometric scale is the evolution of their orientation. The Young–Laplace equation has been employed to obtain an expression for the evolution of the average misorientation angle ($\overline{\theta}$) between adjacent cells by analysing the development of residual stress [11]. An analysis of dislocation glide inside the walls is performed to relate the strain induced within the walls to the total strain. The statistical entropy features as a key element in the analysis as it is related to the pressure induced by dislocations arriving at the walls. The evolution of $\overline{\theta}$ is equal to $\overline{\theta} = \kappa_\theta \gamma^{2/3}$, where $\kappa_\theta = \left(\frac{3}{2}\right)^{1/3}\left(\frac{4\mathcal{N}^{-1}T\Delta S}{\kappa_c \mu b^3 M}\right)^{2/3}$ [11].

When a metal is deformed at a low temperature and a large strain, a different work hardening regime may be observed. This is referred to in the literature as stage IV, and is the stage at which variations in cell size and misorientation become the main contributors to the evolution of the dislocation density [17]. The Young–Laplace equation is applied to stage IV by approximating the dislocation density variation around the cell walls with respect to the misorientation induced by a large amount of deformation [11]. The evolution of the dislocation density at this stage is:

$$\rho_{IV} = \underbrace{\left(\sqrt{\rho_0^*} + \frac{k_{IV}}{2b}\left(\theta - \theta_0^*\right)\right)^2}_{(A')}, \tag{5}$$

where $k_{IV} = \frac{1}{8\kappa_c}\frac{\mu b^3}{\mathcal{N}^{-1}T\Delta S}$, and ρ_0^* and θ_0^* are the dislocation density and misorientation angle at the onset of stage IV, respectively, and are obtained when Eq. (3) and the derivative with respect to γ in Eq. (5) have the same value.

Results for copper single crystals (terms (A) and (B) in Eq. (3)) at different temperatures and strain rates are shown in Figure 1 for (a) the saturation shear stress ($d\rho/d\gamma = 0$) in terms of the homologous temperature $T_h = T/T_m$ and (b) the shear stress–shear strain curves for different temperatures and shear strain rates ($\dot{\gamma} = M\dot{\varepsilon}$), and are compared with experimental data obtained from [19–22]. Table 1 shows the physical parameters employed in the model. It is worth noting that the additional softening behaviour shown in the experiments at 673 and 1223 K is due to dynamic recrystallization [20], an effect not included in the model. Figure 1(c) and (d) shows the model results for the average cell size in polycrystalline copper as functions of temperature and shear strain; the experimental results were obtained from [10] and [23], respectively. The average dislocation density is calculated using Eqs. (3) and (5) for stages I–III and IV ((A') in Eq. (5)), respectively. The large deformation behaviour of polycrystalline copper is shown in Figure 1(e) for the shear stress–shear strain curves when de-

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[2] A_{act} is dimensionless.