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Modelling plastic deformation in BCC metals: Dynamic recovery and cell formation effects

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ABSTRACT

A recently developed model for describing plasticity in FCC metals (E.I., Galindo-Nava, P.E.J., Rivera-Díaz-del-Castillo, Mater. Sci. Eng. A 543 (2012) 110–116; E.I. Galindo-Nava, P.E.J. Rivera-Díaz-del-Castillo, Acta Mater. 60 (2012) 4370–4378) has now been applied to BCC. The core of the theory is the thermostatistical description of dislocation annihilation paths, which determines the dynamic recovery rate of the material. Input to this is the energy for the formation, migration and ordering of dislocation paths; the latter term corresponds to the statistical entropy which features strongly on the solution. The distinctions between FCC and BCC stem primarily from the possible directions and planes for dislocation slip and cross-slip, as well as from the presence of the kink-pair mechanism for dislocation migration in BCC, which are incorporated to the mathematical formulation of the model. The theory is unique in describing the stress–strain response for pure iron, molybdenum, tantalum, vanadium and tungsten employing physical parameters as input; the description is made for wide ranges of temperature and strain rate. Additionally, succinct equations to predict dislocation cell size variation with strain, strain rate and temperature are provided and validated for pure iron.

1. Introduction

Kocks–Mecking (KM) theory has been applied to a wide range of alloys to describe their mechanical behaviour during plastic deformation [23,12,6,40,45–47]. The theory accounts for the competition between the generation and annihilation of dislocations. The corresponding equation describing dislocation density evolution is [37]

$$\frac{d\rho}{d\gamma} = \frac{k_1}{b}\sqrt{\rho} - f\rho, \tag{1}$$

where k_1 is the dislocation storage coefficient, b is the magnitude of the Burgers vector and f is the dynamic recovery coefficient. In general, k_1 and f are obtained by fitting to experimental data to describe the behaviour of specific systems, and it becomes difficult to make predictions or design new materials as the parameters change with composition and microstructure. The factor $(k_1\sqrt{\rho})^{-1}$ accounts for the dislocation mean free path [37]. Modifications to KM model have been made to incorporate additional microstructural effects such as grain size whilst preserving the general form of Eq. (1) [22,21,60,14,20,56].

Previous work by the authors and collaborators [56,26,32,33,41,42] demonstrates that during plastic deformation of metals, a key factor influencing dislocation evolution is the annihilation rate; this is comprised by a dynamic recovery and/or a dynamic recrystallization term. The annihilation rate is usually considered to be a thermally activated process, which energy barrier depends strongly on the annihilation mechanism. A more robust theory is required for obtaining such term from fundamental principles.

Plastic deformation of body centred cubic (BCC) metals occurs by dislocation slip driven by thermally activated kink-pair migration [31,10], leading to dislocation cross-slip for both generation [27] and annihilation [52]. Moreover, the presence of vacancies aids the annihilation of dislocations via their segregation around the dislocation's core enhancing dislocation mobility and climb [11]. At higher temperatures vacancy-assisted dislocation climb becomes the predominant annihilation mechanism [31,36].

In previous work, the dynamic recovery term (f in Eq. (1)) has been derived for pure FCC materials in terms of physical parameters to describe dislocation evolution as a function of temperature and strain rate, as well as the average cell size evolution including stage IV of deformation [26,24,25]. A modified version of the FCC model for plastic deformation and dislocation cell evolution for pure body centred cubic (BCC) metals is presented in this work. The theory is successfully applied to describe the characteristic stress–strain curves of pure Fe, Mo, Ta, V and W at different deformation conditions. The average dislocation cell size evolution of pure Fe is predicted.

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2. Theory

2.1. Kocks–Mecking BCC formulation

Owing to the multiplicity of slip systems, dislocation cross-slip rate is increased in BCC materials compared to FCC [31]: dislocations with $\langle 111 \rangle$ Burgers vector may undergo cross-slip on 48 slip planes: 12 {110}, 12 {112}, and 24 {123} planes, whereas for FCC metals there are only 12 planes for the most likely cross-slip direction [31], it follows that cross-slip events are more frequent in BCC than in FCC metals. Moreover, the number of possibilities for dislocation interaction in BCC metals is lower than for FCC materials as their coordination number (number of possible dislocation interaction directions) is 8 and 12, respectively. These crystallographic characteristics modify the capabilities of BCC materials for dislocation storage and annihilation, increasing the dislocation's mean free path $((k_1\sqrt{\rho})^{-1})$ and the dislocation annihilation rate $(f_{BCC}\rho)$ by a factor of $(48/12)\cdot(8/12)=8/3$. Therefore, it is proposed that in order to describe dislocation evolution for BCC materials, Eq. (1) is modified by increasing the dislocation mean free path and the dynamic recovery coefficient by a factor of 8/3:

$$\frac{d\rho}{d\gamma} = \frac{3k_1}{8b}\sqrt{\rho} - \frac{8}{3}f_{BCC}\rho. \tag{2}$$

2.2. FCC case

The model rests on three assumptions [26]: (i) The velocity v of a dislocation segment is thermally activated and its magnitude can range from zero up to the speed of sound in the material (c); this has been pointed out earlier by Hirth and Lothe [31]. (ii) Once dislocations are in close proximity to each other their strain fields overlap, altering the number of slip paths (microstates) available to the dislocation for displacement; this has been referred to as dislocation impingement [26]. (iii) The energy necessary for a dislocation segment to migrate towards annihilation is proportional to the yield stress of the material (σ_Y) [26,52].

A key feature in this theory is the introduction of the statistical entropy $\Delta S_{FCC} = k_B \ln \Omega_{int}$ that incorporates the possible paths for dislocation motion in terms of the total number of microstates Ω_{int}. In this framework, a microstate is defined as the number of interatomic distances a dislocation segment glides during an arbitrary time step Δt [26]. At high temperatures, where the presence of vacancies becomes relevant, additional microstates are incorporated to account for their interaction with dislocations [24]. When a dislocation segment is considered to move at an average velocity $\langle v \rangle$, the total number of microstates Ω_{int} becomes [26,24]:

$$\Omega_{int} = \Omega_0^{\mathcal{N}} = (\Omega_{dis} + \Omega_{v-d})^{\mathcal{N}} = \left(\frac{\dot{\varepsilon}_0}{\dot{\varepsilon}} + \frac{\vartheta}{\dot{\varepsilon}}\right)^{\mathcal{N}}, \tag{3}$$

where Ω_{dis} and Ω_{v-d} are the number of microstates due to dislocation slip and to vacancy–dislocation interaction, respectively; $\dot{\varepsilon}$ is the strain rate; $\mathcal{N}$ is the impingement effect due to the overlapping strain field of contiguous dislocations that alter the possibilities for dislocation slip (assumption (ii)), and is related to the stacking fault energy of the material [26]:

$$\dot{\varepsilon}_0 = cb\rho_Y \tag{4}$$

is a limiting value for the strain rate, when the material is deformed at the speed of sound; b is the magnitude of the Burgers vector; ρ_Y is the dislocation density consistent with the yield point; and $\vartheta = \vartheta_D \exp(-E_m/RT)$ is the vacancy migration frequency, wherein $\vartheta_D = 10^{13}\ \mathrm{s}^{-1}$ is the Debye frequency, E_m is the vacancy migration energy and R is the gas constant. The transition points where vacancies contribute to dislocation annihilation are obtained by comparing Ω_{dis} and Ω_{v-d} [24]:

- $T_0 = E_m/R\ln(\vartheta_D/\dot{\varepsilon})$, for $\Omega_{v-d} = \vartheta/\dot{\varepsilon} = 1$, when only one vacancy–dislocation interaction microstate is available;
- $T_f = E_m/R\ln(\vartheta_D/\dot{\varepsilon}_0)$, for $\Omega_{v-d} = \Omega_{dis} = \vartheta = \dot{\varepsilon}_0$, when vacancy–dislocation microstates equal those for slip.

For deformation temperatures below T_0 no vacancy effect is present; at deformation temperatures higher than T_f, vacancy-assisted dislocation climb prevails and becomes fully present, and at temperatures between T_0 and T_f, vacancy–dislocation interaction enhances the kink-pair mechanism for dislocation motion.

2.3. Transition temperatures in BCC

T_0 values for pure iron, molybdenum, tantalum, vanadium and tungsten are shown in Table 1 for different strain rate conditions; they are compared with experimental values where the curvature of the flow stress (Fe, Mo), yield stress (Ta, V) and critical resolved shear stress (W) charts significantly change with temperature, decreasing the stress value with increasing temperature, with a corresponding increase in the dislocation annihilation rate. As experimental measurements usually do not show a sharp transition point, some results are shown within temperature ranges where the transitions are observed. The values for E_m were obtained from [59,9,43]. The modelled homologous temperature $T_h = T_0/T_m$ is also shown, where T_m is the melting temperature.

The values of T_0 are in good agreement with the corresponding experimental values (T_0^E) for Fe, Mo and W; for the case of Ta and V the model predictions are below those experimentally measured by ~ 100 K.

2.4. Number of microstates for BCC

The motion of a dislocation in a BCC metal is composed of the migration of two thermally activated kinks; this determines the migration rate necessary for a dislocation to glide [31]. If independent events are considered, this behaviour induces a double kinetic effect for a dislocation to slip, *i.e.* the total number of microstates (Ω) for BCC metals is squared $\Omega = \Omega_{int}\cdot\Omega_{int} = \Omega_{int}^2$. The statistical entropy incorporating the dislocation's kinetic effect then becomes [26,24]:

$$\Delta S_{BCC} = k_B \ln \Omega_{int}^2 = k_B \ln\left(\frac{\dot{\varepsilon}_0 + \vartheta}{\dot{\varepsilon}}\right)^{2\mathcal{N}}. \tag{5}$$

2.5. Dynamic recovery coefficient

Assumption (i) and the multiplicity of dislocation slip paths discussed in the previous subsection lead to an expression for the average dislocation velocity $\langle v \rangle$ for annihilation (expressed in

Table 1
Lower temperature limit.

Material	$\dot{\varepsilon}$ (s^{-1})	E_m (kJ/mol)	T_0^E (K)	Ref.	T_0 (K)	T_h
Fe	8.5×10^{-4}	73.3	250	[8]	245	0.13
Fe	4×10^{-5}	73.3	200–300	[53]	226	0.12
Mo	8.5×10^{-4}	130.2	400–425	[55]	374	0.13
Ta	1.2×10^{-6}	67.5	270–320	[57]	191	0.06
V	2.55×10^{-4}	125.4	500–550	[5]	396	0.18
W	7×10^{-6}	183.3	550–650	[7]	614	0.16