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Rate sensitivity in discrete dislocation plasticity in hexagonal close-packed crystals

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A B S T R A C T

The origin of the rate-sensitive behaviour of plasticity over strain rate regimes from 10^{-5} to 10^{5} s^{-1} has been assessed with reference to three key mechanisms: dislocation nucleation, time of flight (dislocation mobility) and thermally activated escape of pinned dislocations. A new mechanistic formalism for incorporating thermally activated dislocation escape into discrete dislocation plasticity modelling techniques is presented. It is shown that nucleation and dislocation mobility explain rate-sensitive behaviour for strain rates in the range 10^{2} to 10^{5} s^{-1}, but cannot do so for significantly lower strain rates, for which thermally-activated dislocation escape becomes the predominant rate-controlling mechanism. At low strain rates, and for a model Ti alloy considered at 20 °C, the strong experimentally observed rate-sensitive behaviour manifested as stress relaxation and creep is shown to be captured well by the new thermal activation discrete dislocation plasticity model, which otherwise simply cannot be captured by nucleation or mobility arguments. Increasing activation energy leads to a higher energy barrier and as a consequence, a higher dislocation escape time. Conversely, increasing obstacle spacing tends to diminish the thermal activation time.

1. Introduction

The rate sensitivity of the plastic deformation behaviour of alloys has long been of scientific interest and technological relevance, e.g. Refs. [1–4]. Rate sensitivity is strongly material dependent and much work has been done in order to understand its mechanistic basis. Its manifestation is often through the observed progressive increase in flow stress from low strain rates ($\dot{\varepsilon} < 10^3 s^{-1}$) to high strain rates ($\dot{\varepsilon} \geq 10^3 s^{-1}$) in a positively rate sensitive material [5]. It is argued that the plastic deformation is moderated by thermal activation events at low strain rates while being controlled by viscous drag at high rates [6]. Based on the observation of various metals, grain size has also been found to be of influence in rate sensitivity studies [4,7,8] and materials with finer grain structure have been found to be more rate dependent and a coarse grain structure to lead to lower rate sensitivity [9]. Classical time-independent continuum plasticity models assume that the local stress at one material point depends only on the strain at the same point [10]. This theory has been shown to be adequate provided plastic strain gradient effects are small. Where this is not the case, crystal plasticity theory has been developed to incorporate size effects considering plastic strain gradients from the development of geometrically necessary dislocation (GND) densities [11]. However, these theories are based on statistical representations and cannot capture individual local slip events.

Discrete dislocation plasticity (DDP) is a modelling technique in which slip on defined active crystallographic systems is represented through explicit representation and motion of discrete dislocations. In the classical two-dimensional DDP model [12], there are two parameters associated with time scale: first, the dislocation source nucleation time t_{nuc} describes the operation of the Frank-Read source from a trapped dislocation segment to a full, glissile loop, and second, the ratio of viscous drag coefficient and shear modulus B/G characterises the time scale of a dislocation moving within an obstacle-free crystal matrix [13]. A systematic study of rate sensitivity in DDP was conducted by Agnihotri et al. [13] and reveals that quasi-static DDP is able to predict the rate sensitivity in the high strain rate regime of $\dot{\varepsilon} \geq 10^3 s^{-1}$ (albeit only up to rates at which elastodynamic effects become relevant [14]). Beyond $\dot{\varepsilon} = 10^3 s^{-1}$, plasticity is controlled by viscous dissipation and the constitutive rules used in classical DDP models give rise to

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the rate dependence of the material. However, there is no explicit time-associated parameter but rather, the rate sensitivity comes from the strength assigned to obstacles, i.e. the leading dislocation is released from an obstacle immediately once the resolved shear stress exceeds a critical strength, so that classical DDP cannot account for the thermal activation processes particularly at lower strain rates. Thermal activation is thought to be important in the context of enabling the escape of pinned dislocations, for example by obstacles such as solute atoms or small precipitates, simply by the freeing of the pinned dislocation, the development of dislocation jogs, or through dislocation climb. Monnet et al. investigated hardening in a zirconium single crystal using a 3D DDP model in which the mobility of the dislocation is controlled by a kink-pair mechanism [15]. Their model was able to predict the rate sensitivity in the low strain rate regime ($\dot{\varepsilon} < 10^{-3}\mathrm{s}^{-1}$). The analysis was developed using a phenomenological form for the activation free energy associated with dislocation–obstacle interactions based on the body-centred cubic (BCC) crystals study [16]. Hence, their model does not include the dislocation pile-up in front of individual obstacles and no rate sensitivity during nucleation process because new dislocations are introduced using periodic boundary conditions.

Gibbs [17] addressed thermal-activation controlled rate theory based on the concept of thermally-activated escape of pinned dislocations. Gibbs considered a dislocation segment pinned by three obstacles located at two ends and at the segment mid-point. The frequency of successful escape from the middle obstacle was then given in terms of the fundamental frequency with which the pinned segment attempts to overcome (or jump) the energy barriers (lattice vibration) together with the probability of the thermal motion of atoms making a successful attempt. The probability of successful attempts is governed by the Gibbs free energy of activation which allows dislocations to overcome the energy barrier of local obstacles. The Gibbs free energy was expressed as the summation of the Helmholtz energy and the work done by the external stress field, resulting in the establishment of the forward jump frequency of a pinned dislocation under applied stress, and in later utilisation [18], the net jump frequency is given by the difference between the forward and the subsequent reverse jump frequency.

In this paper, we utilise a systematic methodology by considering single crystal stress relaxation in order to study the mechanistic contributions to observed rate-sensitive behaviour over the strain rate regime 10^{-5} to 10^{5} s^{-1}. We address the roles of dislocation nucleation and time of flight or mobility, and present a new formalism for incorporating thermally activated dislocation escape in numerical DDP techniques. We then assess the regimes of strain rate over which each of the mechanisms contribute and predominate, and go on to address the well-known rate-sensitive behaviour of many Ti alloys at 20 °*C* which somewhat surprisingly show remarkable creep and stress relaxation even at low temperature. We finish by assessing the resulting predicted polycrystal rate-sensitive response and show comparisons with experiments.

2. Discrete dislocation plasticity and crystal plasticity formulations

A small-strain, two-dimensional, plane strain discrete dislocation plasticity formulation was developed for hexagonal close-packed (HCP) polycrystals. These crystals in general permit slip along basal, prismatic, and pyramidal *a*-type systems, together with type I and type II pyramidal *c*+*a* systems as detailed in Fig. 1. The plane strain condition imposes the constraint that out-of-plane slip is not permitted and a consequence is a constraint on the slip system activation which is then consistent. In the 2D model considered here, in principle both basal and prismatic *a*-type slip are permitted along with appropriate *c*+*a*-type pyramidal slip which satisfies the plane strain constraint. Here we consider only *a*-prism slip for two reasons: first, the critical resolved shear stress of the *a*-prismatic slip systems is generally lower than that of the pyramidal systems, hence if the loading direction is perpendicular or nearly perpendicular to the c-axis, prismatic slip is always preferred (see Appendix A for detail); second, when the crystal is oriented such that the c-axis is perpendicular to the plane of the DDP model, the set of three *a*-prism slip systems constitutes a linearly dependent set of slip directions that satisfies the plane strain constraint.

Fig. 2 shows schematically a rectangular region with height *H* and width *W*, within which dislocation slip is permitted. The potentially active slip systems are characterised by an angle $\alpha^{(i)}$ with respect to the positive *x*-axis. The three prismatic slip systems are oriented 60° relative to each other, as shown in Fig. 2b. All slip planes are modelled as 100*b* apart. The crystals are taken to be dislocation free initially but with Frank-Read sources randomly distributed on all slip planes. The distribution of obstacles is achieved using the symmetric double-ended model introduced by Chakravarthy and Curtin [19]. The spacing between obstacles on a given slip plane is taken to be uniform. Each source is randomly assigned a nucleation strength τ_{nuc} from a normal distribution of mean value $\overline{\tau}_{nuc}$ and standard deviation $0.2\overline{\tau}_{nuc}$. Edge dislocations only with Burgers vector magnitude *b* can be generated from the sources if the resolved shear stress τ on the source exceeds its strength for a period of time, i.e. nucleation time t_{nuc}, which subsequently glide along the corresponding slip plane. The nucleation time has been estimated by Benzerga [20] and developed by Agnihotri and Van der Giessen [13] as

$$t_{nuc} = \eta_1 \eta_2 \frac{\phi}{\tau b} \tag{1}$$

where 2ϕ is the source length, η_1 is an enhancement factor which describes the dislocation multiplication from semi-ellipse to complete dislocation loop, and η_2 is treated as a constant related to the viscous drag coefficient *B*. The initial length of the dipole is chosen such that the attraction stress between dislocations is equilibrated to the applied stress field τ_{nuc}, thus giving

$$L_{nuc} = \frac{Gb}{2\pi\, \tau_{nuc}(1-\nu)} \tag{2}$$

in which *G* and ν are the shear modulus and Poisson's ratio respectively [12]. For a source with length 2ϕ, its strength can be calculated by τ_{nuc}=Gb/ϕ. The boundary value problem is then resolved utilising the superposition method developed by Van der Giessen and Needleman [12]. Two dislocations on the same plane with opposite Burgers vector annihilate if they are within a critical annihilation distance L_e=6*b*. Dislocation annihilation is modelled by dislocation removal when the annihilation distance is reached. A fixed number of increments is used to resolve the dislocation dynamics at different strain rates. In order to obtain 0.01 strain in 10000 increments, a time step $\Delta t = 1$ ns is required for a strain rate $\dot{\varepsilon} = 10^{3}\mathrm{s}^{-1}$, while $\Delta t = 0.1$ ns is required for $\dot{\varepsilon} = 10^{4}\mathrm{s}^{-1}$; for all strain rates, the change in strain per increment $\Delta\varepsilon$ is fixed. Unless specified, the simulations were performed using the parameters listed in Table 1. The source density and strength were obtained from the fitting of simulated load-deflection responses over a range of specimen sizes to experimental micro-cantilever data for α-Ti [21] in Tarleton et al. [22]. The model was validated by comparison with pure bending tests carried out by Cleveringa et al. [23]. All the single crystal studies were performed using the reference crystal orientation, i.e. $\alpha^{(1)}$=0°.