

ON A DISLOCATION-BASED CONSTITUTIVE MODEL AND DYNAMIC THERMOMECHANICAL CONSIDERATIONS

J. C. Nieto-Fuentes*, D. Rittel and S. Osovski

Faculty of Mechanical Engineering, Technion, 32000 Haifa, Israel

ABSTRACT

Dislocation-based constitutive models are widely used to predict the plastic behavior of metallic materials, in both quasi-static and dynamic conditions. In addition, if the ratio of (adiabatic) thermomechanical (plastic work to heat) conversion is known, the stress-strain-temperature relationship can be estimated. The main purpose of this study was to verify the applicability of a widely-used expression (where the strain energy of a plastically deformed material is proportional to the density of dislocations) to calculate the stored energy in the material, which can be used in parallel with the micromechanical model to estimate the temperature rise during dynamic plastic deformation. An experimental campaign, where Kolsky (split Hopkinson) pressure bar tests were combined with *in situ* infrared temperature measurements, was conducted on OFHC copper compression specimens. The analytical thermomechanical conversion was compared with the experimental one, revealing *a significant discrepancy between the two*. An empirical *ad hoc* factor was introduced in the analytical expression in order to describe adequately the thermomechanical response of the material under dynamic (impact) loading conditions.

* Corresponding author at: Faculty of Mechanical Engineering, Technion, 32000 Haifa, Israel.

Tel: +972 58 658 1100

E-mail address: juan-carlos@campus.technion.ac.il (Juan Carlos Nieto Fuentes)

HIGHLIGHTS

- Kolsky (impact) experiments were performed on cylindrical OFHC Cu specimens.
- *In situ* temperature measurements during impact testing were conducted.
- A dislocation-based constitutive model was used to define the dynamic response.
- The analytical and experimental Taylor-Quinney factors (TQFs) differ significantly.
- An *ad hoc* factor was added to calculate the strain energy and the TQF.

KEYWORDS

Taylor-Quinney coefficient. Dislocations (A). Rate-dependent material (B). Constitutive behavior (B). Kolsky bar (C).

1. Introduction

One of the first attempts to predict the plastic behavior of materials based on dislocation-mechanics constitutive relations was developed by Taylor (1934), followed by many others (Gil Sevillano et al., 1980; Kocks and Mecking, 2003; Kuhlmann-Wilsdorf, 1989; Mughrabi, 1987; Nabarro et al., 1964; Nes, 1998; Zerilli and Armstrong, 1987). In the general theory of work-hardening, stresses are given as a function of the dislocation density, *e.g.* the shear flow stress of a single crystal is given by the expression (Bailey and Hirsch, 1960; Cottrell, 1953; Kuhlmann-Wilsdorf, 1989):

$$\tau = \tau_0 + \alpha Gb\sqrt{\rho_{tot}} \quad 1-1$$

where α is a constant between 0.25 and 0.5, τ_0 is the critical resolved shear stress, G is the shear modulus, b is the Burgers vector and ρ_{tot} is the total line dislocation density. This expression, which is universally applied in dislocation-based constitutive models, can be multiplied by the Taylor factor M to obtain the uniaxial flow stress - $\sigma = M\tau$ - in a polycrystalline material. Commonly, M is approximated to 3.06 for most FCC metals (Kocks, 1970).

Under impact loading conditions, *i.e.* high strain rate deformation, a notable temperature rise is expected – due to the prevalence of nearly adiabatic conditions (Boley and Weiner, 1997).

The energy balance (or heat conduction) equation, coupled with the mechanical heat source under high strain rate deformation, is expressed as:

$$\lambda \nabla^2 T - \alpha_v \frac{E}{1-2\nu} T_0 \text{tr}(\dot{\epsilon}^e) + \beta_{diff} \sigma_{ij} d\dot{\epsilon}_{ij}^p = \rho C \dot{T} \quad 1-2$$

where the three terms in the left hand side are related to heat conductance, reversible thermoelastic heating, and irreversible thermoplastic heating, respectively. λ is the thermal conductivity, α_v is the volumetric thermal expansion coefficient, E stands for Young's modulus, ν is Poisson's coefficient, T_0 is the initial or ambient temperature, $\dot{\boldsymbol{\varepsilon}}^e$ is the elastic strain rate tensor, while σ_{ij} and $\dot{\boldsymbol{\varepsilon}}_{ij}^P$ are the components of the stress and the plastic strain rate tensors, respectively. Here we remark that the term β_{diff} is the differential form of its integral counterpart, the Taylor-Quinney coefficient, that will be later detailed. On the right hand side of Equation 1-2, ρ is the material density and C is the heat capacity. The overdot in both sides of the expression stands for differentiation over time. Commonly, the temperature rise related to the thermoelastic coupling effect does not exceed 0.2 °C for metals (Bever et al., 1973), and can thus be neglected when compared with the thermoplastic heating. In addition, when adiabatic conditions predominate, the term $\lambda \nabla^2 T = 0$. As a result of the previous assumptions, and solving Equation 1-2 for the Taylor-Quinney coefficient (ratio of the thermomechanical conversion) in its integral form (Rittel, 1999):

$$\beta_{int} = \frac{\rho C \Delta T}{\int \sigma_{ij} d\varepsilon_{ij}^P} = \frac{\rho C \Delta T}{\int dW_p} \quad 1-3$$

where ΔT is the increment of temperature during deformation and W_p corresponds to plastic work. Bever et al. (1973) made an extensive review in the conversion of mechanical into thermal energy during plastic deformation. During the past years, many works focusing on failure mechanisms under high loading rates, have proposed that the temperature rise contributes significantly to the onset of failure due to thermal softening (Khan et al., 2004; Ma et al., 2012; McAuliffe and Waisman, 2015; Zhang et al., 2016). When the value of β_{int}

approaches 1, most of the plastic work is dissipated through heat and almost no energy is stored in the material. In light of the numerous microstructural observations, where significant amount of dislocations were observed to accumulate in the deformed materials (often leading to microstructural rearrangement) one may expect the β_{int} value to be smaller. In fact, Rittel et al. in their work on single crystalline tantalum (Rittel et al., 2009) have reported values ranging from 0.4-1 depending on the crystallographic orientation of the deformed specimen. Other measurements of β_{int} in the literature, covering a large range of both metallic and polymer materials (Bjerke et al., 2002; Ghosh et al., 2017; Hodowany et al., 2000; Macdougall and Harding, 1998; Mason et al., 1994; Rittel, 1999; Rittel et al., 2017, 2012), showed that the fraction of work converted into heat during high strain rate deformation is not always roughly 1, and can range from 0.3 to 1, depending on the material and the microstructure. For OHFC copper, Rittel et al. (2012) have demonstrated the role of grain boundaries in increasing the amount of stored energy by comparing polycrystalline and single crystal specimens. It is worth mentioning here the numerical modeling work of Benzerga et al. (2005), who used a two-dimensional dislocation dynamics approach to calculate the stored energy of cold work (SECW) and reported that the Taylor-Quinney factor can reach values of up to 0.7 – at least at low plastic strains (less than 0.1).

Kapoor and Nemat-Nasser (1998) measured the increase of temperature during high strain rate plastic deformation in Tantalum-2.5%W alloy. Besides, they calculated the energy stored in the material based on the stress field around a dislocation, using the well-known expression derived from elasticity (Bacon and Hull, 2011; Hirth and Lothe, 1982) - which can be approximated as:

$$E_{stored} = \alpha G b^2 \rho_{tot} \quad 1-4$$

and substituted in Equation 1-3 applying the first law of thermodynamics, to obtain:

$$\beta_{int} = \frac{\rho C \Delta T}{\int dW_p} = \frac{\int dW_p - E_{stored}}{\int dW_p} \quad 1-5$$

While the temperature measurements of Kapoor and Nemat-Nasser (1998) for impacted Ta2.5%W gave a value of β_{int} close to 0.7, the analytical calculation brought a value of 0.995, so that a fraction of 0.5% of the total energy invested in the deformation remains stored in the material as microstructural defects. The authors attributed this discrepancy to the lack of accuracy of the temperature measurement technique, *i.e.* the infrared (IR) detector. In view of the numerous temperature measurements cited above, where a large range of β_{int} were reported, the experimental findings of Kapoor and Nemat-Nasser (1998) fall within the plausible range of values. On the other hand, the analytical expression they used is widely known and is often being used in the literature. Here, we may ask ourselves: who is to blame? To address this question, *it appears reasonable to clarify whether Equation 1-4 – a universal expression that can be used to calculate the stress-strain response of the material – is equally adequate to estimate the strain energy storage of a dynamically deformed material.* While that point has been implicitly taken for granted, it has not been verified systematically so far, to the best authors' knowledge.

To use Equation 1-4, a reliable model accounting for the evolution of the total dislocation density is required. In 1998, Estrin et al. (1998) have suggested a dislocation-based model for all hardening stages (ETMB model). In their model (Estrin et al., 2006, 1998; Toth et al., 2002), a dislocation cell structure is formed during straining of the material, which consists

of two different phases: one corresponding to the cell interior and, surrounding it, the one belonging to the cell wall. The model proposes a phenomenological approach to describe the mechanical behavior of crystalline materials at large strains, both in 2D and 3D. The ETMB model, has been proven itself repeatedly for various materials and loading scenarios. Mckenzie et al. (2007) modified the model to make it applicable for processes of severe plastic deformation (SPD) under hydrostatic pressure. Lemiale et al. (2011, 2010) combined the ETMB model with finite element (FE) calculations to simulate grain refinement in the material under high strain rate loading, such as metal particle impact. Ding and Shin (2011) and Ding et al. (2011) used a similar approach to model the microstructural evolution during machining of aluminum 6061, OFHC copper and commercially pure titanium. Atmani et al. (2015) used the ETMB model to characterize the grain size evolution during OFHC copper machining. Rittel and Osovski (2010), in an attempt to study dynamic recrystallization (DRX) within adiabatic shear band (ASB) formation, have used the model to describe the microstructural rearrangement leading to DRX.

In order to give a more physical perspective to the model, Parvin and Kazeminezhad (2014) introduced the effect of the stacking fault energy (SFE), which is a microstructural material parameter that affects the dynamic recovery (annihilation) rate during deformation. The effect of storage and annihilation of dislocations during plastic deformation is reflected in different stages of work hardening, as reviewed by Rollett and Kocks (1993). The SFE has likewise an influence in the mobility of dislocations. As the SFE is lower, the activation energy for cross slip and thus the difficulty of forming cell structures in the material, is higher (Landau et al., 2009). Moreover, studies on brass indicate that a decrease in the SFE leads to

a decrease in the grain size and an increase in the densities of dislocations and deformation twins (Wu et al., 2013). Following the work of Parvin and Kazeminezhad (2014), Liu et al. (2016) modified the expression used to predict the evolution of the cell size, introducing a new coefficient based on material properties and not determined by fitting experimental data, which gives more physical consistency to the problem.

Additionally, one direct consequence of the accumulation of dislocations due to plastic deformation is the increase of the misorientation angle between dislocation cells, which leads to a microscopic non-uniform deformation – even though the material may be uniformly deformed from a macroscopic point of view (Needleman and Sevillano, 2003). The concept of geometrically necessary dislocations (GNDs) was introduced to designate those dislocations that appear to accommodate the lattice curvature during deformation (Ashby, 1970; Gao and Huang, 2003; Nye, 1953). The last version of the ETMB model (Estrin et al., 2006), developed in 2006 by several of the original authors, also included this population of dislocations, and provided a way to calculate the misorientation angle between adjacent cells. In spite of this progress, few authors included this modification in their works.

The large amount of successes in using the ETMB model, have led us to rely on it for estimating the evolution of the dislocation density in a dynamically deformed material. The ETMB model, modified to a small extent, is used to analytically assess the amount of stored energy in the material following impact loading, using Equation 1-4.

In addition, experimental work was carried out to measure and introduce in the model the effect of the thermomechanical conversion during deformation. The experimental results, *i.e.*

the measured value of β_{int} throughout the deformation process, were then compared with the analytical assessment.

Hereinafter, in the first part of the paper we briefly explain the experimental procedure and materials. Afterwards, the analytical model and the modifications introduced are described. The next section examines the main results, to be discussed thereafter. Our conclusions of the work are finally presented.

2. Experimental methods

2.1. Material and specimens

The specimens used during the experimental campaign were compression cylinders machined from a $\Phi 12$ mm rod of polycrystalline oxygen free high-conductivity (OFHC) copper, in as-received condition. Samples for scanning electron microscopy were cut from the as-received rod. Following standard polishing techniques, the specimens were subjected to EBSD analysis using an Oxford EBSD detector in a Tescan MIRA-3 FEG SEM. The EBSD image and inverse pole maps are given in Figure 2-1. The average grain size was determined to be $36\text{ }\mu\text{m}$. The specimens were precisely machined with different lengths and diameters, to control the applied strain rate: L4 Φ 4 (2 samples tested at 5400 s^{-1}), L5 Φ 5 (4 samples tested at 4400 s^{-1}) and L6 Φ 6 (3 samples tested at 3500 s^{-1}).

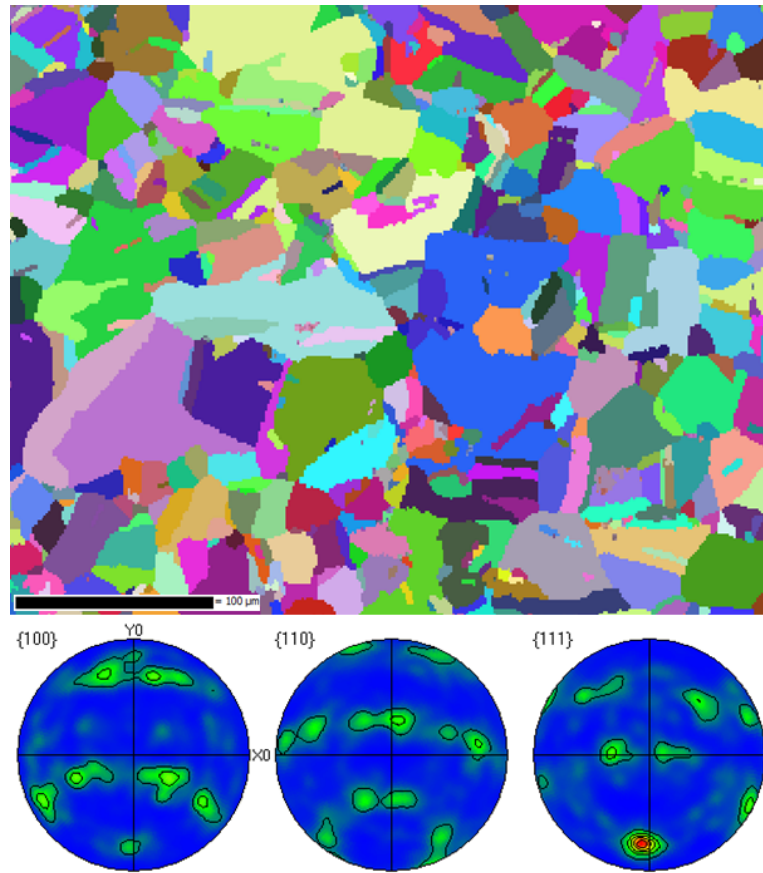


Figure 2-1. Grain map distribution and pole figures, obtained from EBSD analysis.

2.2. Experimental setup

Kolsky bar – High strain rate compression experiments were performed at room temperature (295K) using a split Hopkinson pressure bar (SHPB). First introduced by Kolsky (1949), the main principle of this experimental technique is the one dimensional propagation of elastic stress waves, whose specific formulation is provided elsewhere (Meyers, 1994). As can be seen from Figure 2-2, the specimen is placed in between two $\Phi 19.36$ mm C300 maraging steel bars. The striker is then propelled by compressed air before hitting the end of the incident bar, generating an elastic pulse - incident wave - that travels through the bar until it

reaches the specimen. Part of the incident wave is reflected back to the incident bar with opposite sign – reflected wave – and part passes through the specimen, deforming it plastically, into the transmitter bar – transmitted wave.

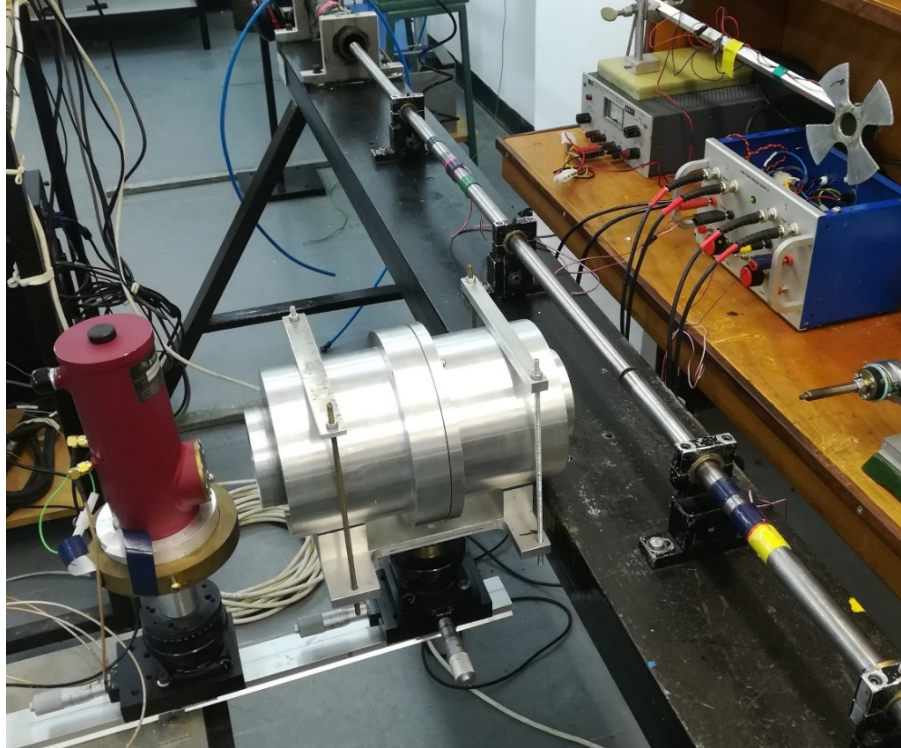


Figure 2-2. Experimental setup for thermal and mechanical measurements during Kolsky tests.

Temperature measurements – In parallel, to calculate the response during the experiments, *in situ* high speed temperature measurements – using an infrared detector – were conducted. Infrared radiation is transformed by the detector into an electric signal, which is proportional to the collected radiation. The detector used during the experimental campaign is based on two photoconductors (InSb & HgCdTe), each one operating on a different wavelength, with an active element area of 250x250 μm . They exhibit a very fast response, suitable for short time events, as the ones considered in this work. To prevent noisy signals, the detectors are cooled at cryogenic temperatures (using a liquid N_2 pour-filled Dewar flask). The InSb

photodiode of our infrared detector covers the spectral range from 1 to 5.5 μm (short to mid-wavelength infrared), whereas the HgCdTe element detects radiation from a wavelength of 5.5 to 12 μm (mid to long-wavelength infrared). Using Wien's displacement law, one can calculate the range of temperature in which the detector can collect the radiation emitted from the specimen, just by substituting the wavelength peaks under consideration. Thus, in the case being discussed, the operating temperatures fall in the range of 241K-2898K.

To concentrate the radiation emitted from the specimen in the focal point of the detector, a reflective optical system is used – see in Figure 2-2 the cylindrical aluminum case between the IR detector and the specimen. The system is a modification of the classical Schwarzschild two-mirror configuration. In this case, a four-mirror configuration, already presented by Rittel and Wang (2008), prevents the central obstruction caused if the detector is placed between the specimen and the optical system.

The *calibration* procedure consisted on heating a dummy specimen of the same material, placed on the tip of a soldering iron. Since the detector gives a voltage signal, which is proportional to the measured radiation, a relation between the signal and the temperature is needed. For that purpose, a K-type thermocouple is embedded in the calibration sample. During cooling of the soldering iron to room temperature, both signals – IR detector and K-type thermocouple – are recorded simultaneously. To insure repeatability, the calibration curves were measured multiple times (≥ 5); then, a relation between both signals can be obtained (see an example in Figure 2-3). Since the thermocouple itself is a voltage-temperature transducer, the difference in temperature can be finally calculated.

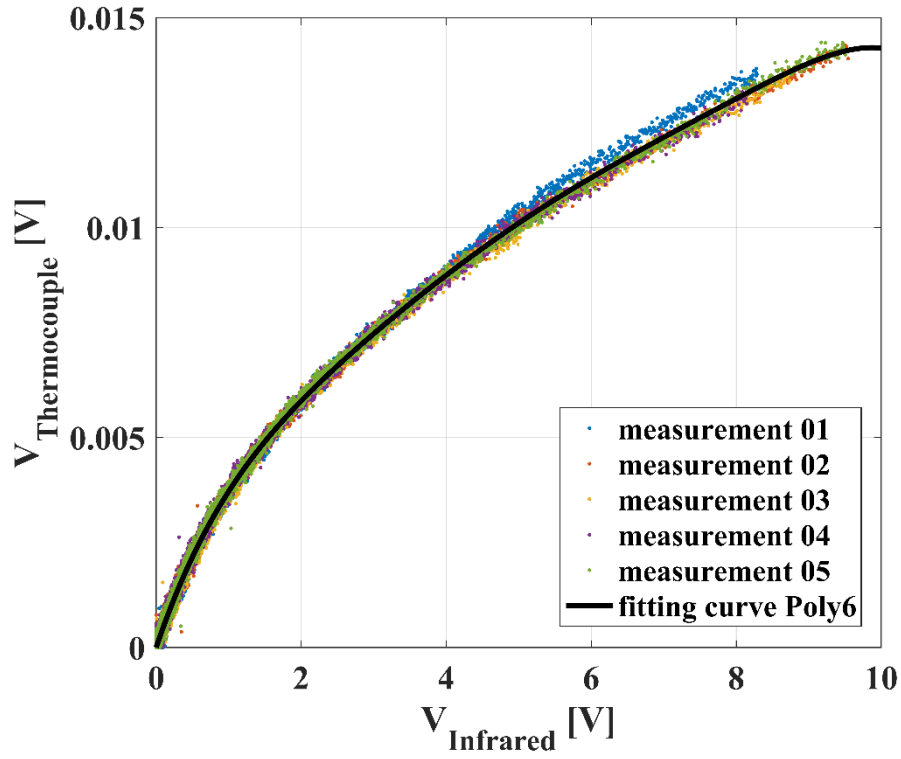


Figure 2-3. K-type thermocouple signal vs. infrared detector signal. The fitting curve was chosen as a sixth-degree polynomial.

The increase of temperature measured during the experiments enables the determination of the Taylor-Quinney factor, using Equation 1-3.

3. Model

Material model - In the framework of the dislocation density-based model developed by (Estrin et al., 2006, 1998) and Toth et al. (2002), and the subsequent modifications conducted by other authors (Liu et al., 2016; Parvin and Kazeminezhad, 2014), the model presented here combines those physical assumptions that provide an insight on the dynamic (high strain rate) behavior of metallic materials deformed at low strains. The principal expressions and

the main assumptions of the model are given in this section; for additional details, the reader is referred to Appendix A.

The model itself considers the material to be divided into two different, but dependent phases: *cell walls*, with a high dislocation density, and *cell interiors*, practically free of dislocations in comparison with the walls. Using an empirical rule, the evolution of the cell and the dislocation density can be estimated during deformation. Thus, the glide resistance of the cell can be calculated as the weighted resistance of the cell interiors and the cell walls, depending on the volume that the latter occupy in the overall structure. Hereafter, the definition of the total dislocation density – which will be used in the calculation of the stored energy - is defined by the rule of mixtures (Estrin et al., 2006, 1998; Rittel and Osovski, 2010; Toth et al., 2002):

$$\rho_{tot} = f(\rho_w + \rho_{GND}) + (1 - f)\rho_c \quad 3-1$$

where ρ_w is the line dislocation density of the cell walls, ρ_c is the line dislocation density of the cell interiors, and ρ_{GND} is the line dislocation density of GNDs that accumulate in the walls (and contribute to the misorientation). The volume fraction of the cell walls, f , is to be understood as a geometrical parameter that relates the thickness of the walls with the width of the cell; a schematic representation can be found in Figure 4 of (Estrin et al., 1998). During deformation, the dislocations tend to bunch together in the walls, these becoming narrower and narrower. The evolution equation of the volume fraction can be defined as:

$$f = f_\infty + (f_0 - f_\infty) \exp\left(\frac{-\gamma}{\gamma_0}\right) \quad 3-2$$

being f_∞ the saturation value at large strains, f_0 its peak value and γ_0 its rate of decrease. As can be seen, f decays with the resolved shear strain γ , meaning that the thickness of the wall decreases as strain increases, **as already stated**. The dislocation densities of both the cell walls and cell interiors are influenced by basically three phenomena: generation of dislocations by Frank-Read sources (subscript FR), migration of dislocations from cell interiors to cell walls (subscript M) and dynamic recovery (subscript A). **Here, we adopted the simpler two-dimensional version of the ETMB model (Estrin et al., 1998) for the generation and migration terms, with a slight modification for the annihilation terms as suggested by (Huang et al., 2009; Parvin and Kazeminezhad, 2014) – as will be discussed later in this section. In the absence of *in situ* dislocation density measurements, the initial dislocation density of the cell walls and the cell interiors at the beginning of the deformation was assumed to be 10^{10} m^{-2} , an intermediate value among those found in (Estrin et al., 1998) and (Hirth and Lothe, 1982). As a function of the increasing strain, the evolution of the dislocation density in the cell walls can be defined as:**

$$\left(\frac{d\rho_w}{d\gamma} \right) = \left(\frac{2\beta^*(1-f)\sqrt{\rho_w + \rho_{GND}}}{bf\sqrt{3}} \right)_{FR} + \left(\frac{4\beta^*\sqrt{1-f}}{bdf}(1-\xi) \right)_M - \left(\frac{1}{\dot{\gamma}} \frac{Gb^4\rho_w\mathcal{G}_D}{\pi V\Gamma} \exp\left(-A \ln\left(\frac{Gb^4\mathcal{G}_D}{16\pi V\Gamma\dot{\gamma}} \right) + \frac{\tau_w V}{Gb^3} \right) \right)_A \quad 3-3$$

where β^* is a constant that determines the fraction of dislocations that can enter the walls, ξ is the fraction of dislocations that contribute to increase the misorientation between cells (further explained in Appendix A), $\dot{\gamma}$ is the shear strain rate, $\mathcal{G}_D$ is the Debye frequency, V is the activation volume for cross-slip, A is a constant related with the stacking fault energy

of the material – Γ – and approximately equals to 1, and τ_w is the glide resistance of the cell wall, which is defined as (Lemiale et al., 2010; Rittel and Osovski, 2010):

$$\tau_w = \alpha G b \sqrt{\rho_w} \left(\frac{\dot{\gamma}}{\dot{\gamma}_0} \right)^{\frac{T}{T_m}} \quad 3-4$$

being $\dot{\gamma}_0$ a reference shear strain rate and T_m the melting temperature of the material. The selection of the reference shear strain rate should be in accordance with an upper limit of the characteristic velocity of deformation, *i.e.* a typical value for quasi-static deformation may be 1 s^{-1} , while a reference shear strain rate of 10000 s^{-1} may be characteristic of medium-to-high strain rate deformation (Rittel and Osovski, 2010). The size of the new formed dislocation cells, d , can be calculated using the following formula (Holt, 1970):

$$d = K / \sqrt{\rho_{tot}} \quad 3-5$$

where K is the so-called proportionality coefficient (see Appendix A for additional details), usually assumed constant by many authors.

Turning our attention now to the annihilation term in the cell walls, we want to remark that the mechanism for recovery here cannot be thermally activated under **nearly** adiabatic conditions – resulting from the low increase of temperature observed during the experimental campaign (see experimental results) together with the characteristic short time scales. Instead, pairwise annihilation of dislocations by cross-slip is considered (Estrin et al., 1998; Toth et al., 2002), adopting as a reference the expression developed by Huang et al. (2009) and included by Parvin and Kazeminezhad (2014) in their model. Here, assuming that the probability of cross-slip attempt in the cell walls is higher than that in the cell interiors as a

result of the higher density (see Results section), the influence of increasing the recovery term on the strain hardening response was studied. Interestingly, based on the work-hardening behavior of the material during the experiments, this term should be increased at least eight times compared with the original one (see Equations 3-3 and 3-6 for a comparison between the primitive and the modified annihilation term).

In a similar way as in Equation 3-3, although conserving the original recovery term in (Parvin and Kazeminezhad, 2014), the evolution of the dislocation density in the cell interiors can be defined as:

$$\left(\frac{d\rho_c}{d\gamma}\right) = \left(\frac{2\alpha^*}{3\sqrt{3}} \frac{\sqrt{\rho_w + \rho_{GND}}}{b}\right)_{FR} - \left(\frac{4\beta^*}{bd\sqrt{1-f}}\right)_M - \left(\frac{1}{\dot{\gamma}} \frac{Gb^4 \rho_c \mathcal{G}_D}{8\pi V \Gamma} \exp\left(-A \ln\left(\frac{Gb^4 \mathcal{G}_D}{16\pi V \Gamma \dot{\gamma}}\right) + \frac{\tau_c V}{Gb^3}\right)\right)_A \quad 3-6$$

where α^* stands for the fraction of operative sources, and τ_c the glide resistance of the cell interiors, defined as:

$$\tau_c = \alpha Gb \sqrt{\rho_c} \left(\frac{\dot{\gamma}}{\dot{\gamma}_0}\right)^{\frac{T}{T_m}} \quad 3-7$$

Regarding the migration term in this case is negative, corresponding to the dislocations that leave the cell interiors and join the walls. The recovery term corresponds to the original formulation in (Parvin and Kazeminezhad, 2014), based on dislocation annihilation by cross-slip. Once both expressions to define the shear strength of the cell interiors and the cell walls are described (Equations 3-4 and 3-7), the resulting shear flow stress can be calculated as:

$$\tau = f\tau_w + (1-f)\tau_c \quad 3-8$$

As commented in the introduction with respect to Equation 1-1, multiplying Equation 3-8 by the Taylor factor, and adding the yield stress of the material, σ_0 , the uniaxial flow stress can be obtained:

$$\sigma = \sigma_0 + M\tau \quad 3-9$$

Upon fitting the analytical stress strain curve to the experimentally measured one, the plastic work and amount of stored energy as a function of strain can now be calculated.

Thermal considerations - As mentioned in Section 2, temperature measurements during high strain rate deformation of OFHC copper were performed. The increase of temperature related to each increment of strain is introduced in Equation 1-3 to calculate the experimental β_{int} . This value is then compared with the analytical one (β_{int}^*), which can be calculated using Equation 1-5 in the following way:

$$\beta_{int}^* = \frac{\int dW_P^* - E_{stored}}{\int dW_P^*} \quad 3-10$$

where W_P^* corresponds now to the analytically calculated plastic work. The dissimilarity between both (analytical and experimental) thermomechanical ratios can be used to introduce in the model an additional physical phenomenon associated with plastic deformation at high strain rates, *i.e.* the increase of temperature.

4. Results

4.1. On the σ - ε_p relationship

Dislocation density-based constitutive models are highly sensitive to the selection of the suitable parameters, which can thoroughly represent the material behavior under different scenarios. Table 4-1 summarizes the material parameters and model constants used to define the plastic behavior of OFHC copper under high strain rate loading conditions (those parameters not explained heretofore can be found in Appendix A).

Table 4-1. Material parameters and constants for OFHC copper (SI units if applicable).

Parameter	Value [units]	Reference
α	0.33	adjusted
α^*	0.0022	adjusted
β^*	0.008	adjusted
γ_0	1	(Rittel and Osovski, 2010)
$\dot{\gamma}_0$	10^4 s^{-1}	(Rittel and Osovski, 2010)
Γ	0.06 J/m^2	(Landau et al., 2009)
κ	1.85	(Liu et al., 2016)
ν	0.345	(Simon et al., 1992)
θ_0	0.1745 rad	(Rittel and Osovski, 2010)
$\mathcal{G}_D$	10^{13} s^{-1}	(Liu et al., 2016)
ρ	8900 kg/m^3	(Simon et al., 1992)
$\rho_{c,initial}$	10^{10} m^{-2}	adjusted
ρ_m	10^{14} m^{-2}	(Liu et al., 2016)
$\rho_{w,initial}$	10^{10} m^{-2}	adjusted
A	1.05	(Meyers et al., 1997)
b	$2.56 \times 10^{-10} \text{ m}$	(Simon et al., 1992)
c	3810 m/s	(Liu et al., 2016)
C	$385 \text{ J/kg}\cdot\text{K}$	(Simon et al., 1992)
E_m	87000 J/mol	(Liu et al., 2016)
f_0	0.25	(Estrin et al., 1998; Toth et al., 2002)
f_∞	0.06	(Estrin et al., 1998; Toth et al., 2002)

G	47.4x10 ⁹ Pa	(Simon et al., 1992)
k	1.38x10 ⁻²³ J/K	-
K_I	25	(Liu et al., 2016)
M	3.06	(Kocks, 1970)
R	8.134 J/molK	-
T_m	1356 K	(Simon et al., 1992)
V	300b ³	(Parvin and Kazeminezhad, 2014)

Among the several parameters presented above, a parametric study over α^* and β^* was performed, to determine the influence of the dislocations generation mechanisms in cell interiors and walls. Indeed, the values resulting from this study, even though they deviate from those reported by other authors, do fall into their boundaries (Ding and Shin, 2011; Estrin et al., 1998; Liu et al., 2016; Parvin and Kazeminezhad, 2014; Rittel and Osovski, 2010; Toth et al., 2002). Figure 4-1 shows a comparison between the averaged experimental stress vs. plastic strain curves and the model prediction, for the three different strain rates. The curves are presented with standard error (standard deviation of the sample mean) bars and the y axis is magnified for the sake of visualization. The repeatability of the experimental results for each strain rate was observed. The mechanical behavior of OFHC copper appeared to be strain rate sensitive, since the higher the strain rate, the higher the work hardening.

Note that the dynamic response of the material at small plastic strains was not fully captured by the model; the experimental curves exhibit a sudden increase of stress until a plastic strain of 0.05, while the model prediction is underestimating the initial strain hardening. A similar observation was made by Lemiale et al. (2010) when using the ETMB model for a high strain rate scenario.

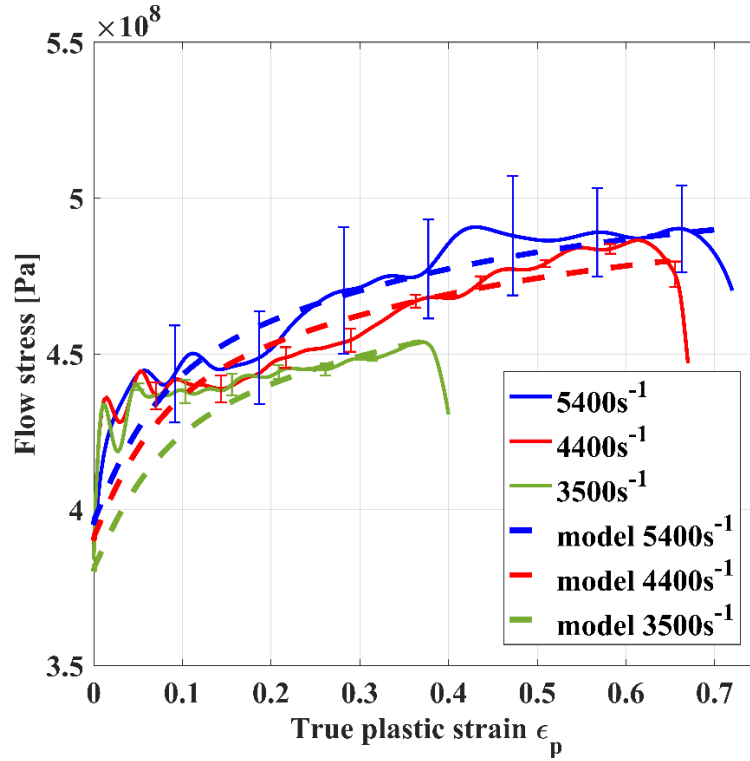


Figure 4-1. Comparison between averaged experimental and predicted σ - ϵ_p curves. Standard error (SE) bars are shown.

Regarding the variation of the density of dislocations during deformation, Figure 4-2 illustrates the evolution of the different populations of dislocations considered throughout this work; as an example, the loading case at a strain rate of 5400 s^{-1} is shown. Here it is essential to note the comparable evolution pattern for the different strain rates, *i.e.* the dislocation density in the cell walls is dominant throughout the deformation, being at least one order of magnitude higher than that of the cell interiors. Additionally, we observed a swift increase in the dislocation densities at strains lower than 0.1, where the annihilation terms are still a negligible phenomenon in the deformation process. After this point, the growth of dislocation densities in the cell walls and cell interiors tends to stabilize, being less remarkable for the case of geometrically necessary dislocations – which are assumed to be

unrecoverable – increasing in density without bounds thus enlarging the misorientation angle between sub-grains (Estrin et al., 2006).

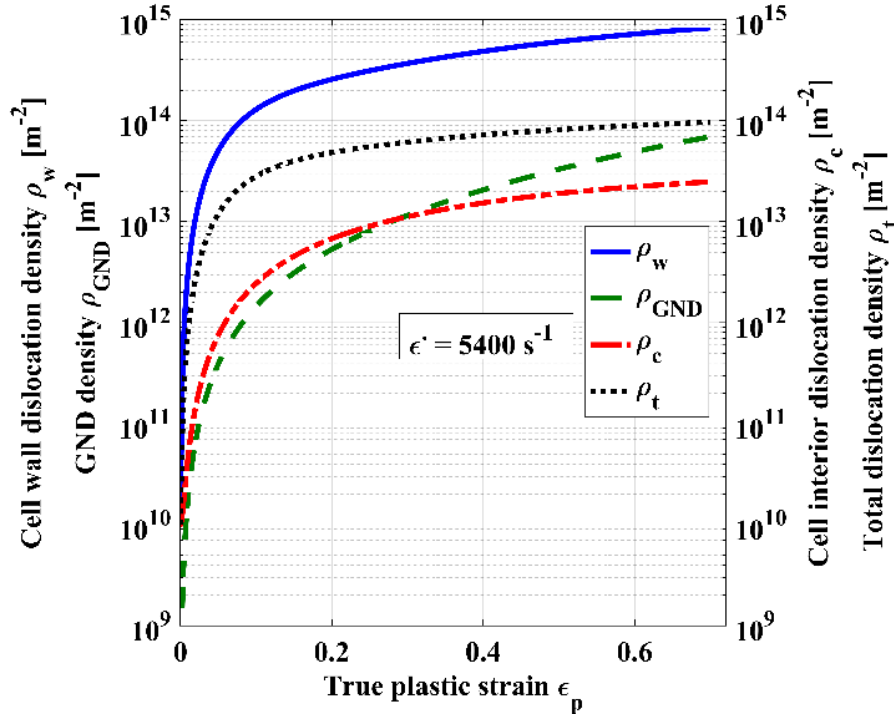


Figure 4-2 - Evolution of the different dislocation densities with strain (strain rate of 5400 s^{-1}).

4.2. On the stored energy of cold work

Figure 4-3a shows the typical record of the temperature increase during the tests. Here, the voltage signal corresponding to the radiation collected by the infrared detector is already converted into temperature rise. The calibration procedure to accomplish such conversion was already detailed in Section 2.2, as in (Rittel et al., 2012, 2007). At first, the signal oscillates around a mean value equal to zero, until at some point the temperature rise starts to evolve. To simultaneously adjust the temperature recording with the stress-strain response of the material, one ought to determine the time span between the data recording outset and the stress wave travelling time through the incident bar, before attaining the specimen; *e.g.*

in Figure 4-3a the synchronization started at 162 μs , until the end of the deformation at approximately 277 μs . After the latter point, the specimen may be subjected to multiple impacts on account of the stress wave travelling back and forth through it, which are not considered as part of the test. **Let us remind here that an earlier analysis of the transient temperature distribution throughout a cylindrical specimen, indicated that the dimensions of the specimens used (comparable with the ones in this study) guarantee the homogeneous deformation and temperature distribution all over the specimen (Rittel and Rabin, 2000).**

Figure 4-3b shows the actual experimental increase of temperature versus plastic strain for the same specimen, in addition to the analytical prediction for a specimen deformed at the same strain rate – here, all the plastic work was considered to be converted into heat ($\beta_{int}=1$).

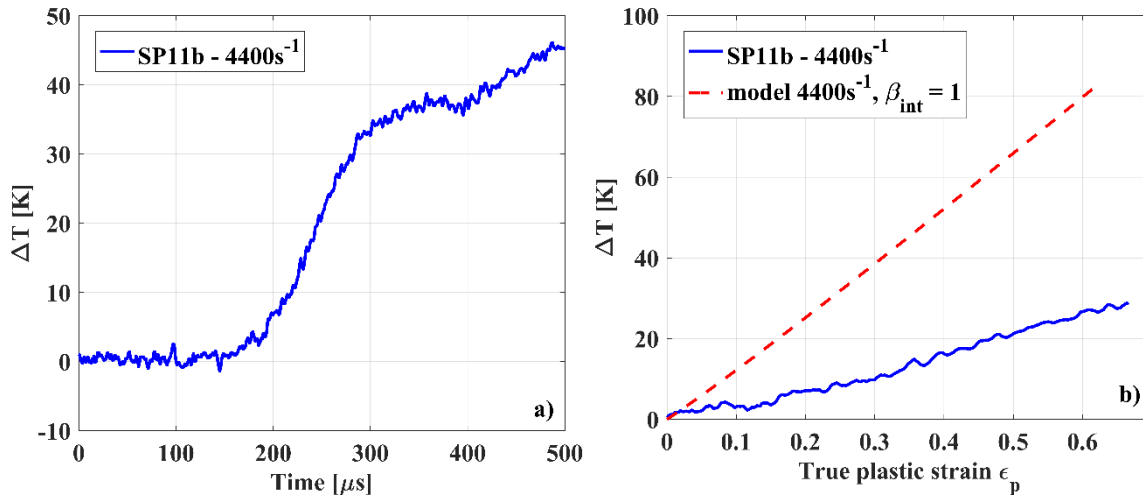


Figure 4-3. a) Typical temperature increment record during experiments. Specimen SP11b, deformed at 4400 s^{-1} . b) Comparison between the experimental increase of temperature during deformation and the model prediction (using $\beta_{int}=1$).

Therefore, introducing the experimental temperature rise and the stress-strain response of the material in Equation 1-3, the experimental ratio of thermomechanical conversion (β_{int}) was calculated. Figure 4-4 illustrates the averaged evolution of β_{int} with plastic strain for the three

different strain rates. Note that a strain rate dependency of the thermal factor cannot be established here, in contrast to the results of other authors for the same material (Rittel et al., 2012). Accordingly, the reduction of the three curves into one, that may exhibit a generic thermal response of OFHC copper under high strain rate loading, was done – see the dashed curve in Figure 4-5. Besides, one can calculate the fraction of energy stored in the material, namely the stored energy of cold work (SECW) (Bever et al., 1973), just by calculating $(1 - \beta_{int})$ – see the solid line in Figure 4-5.

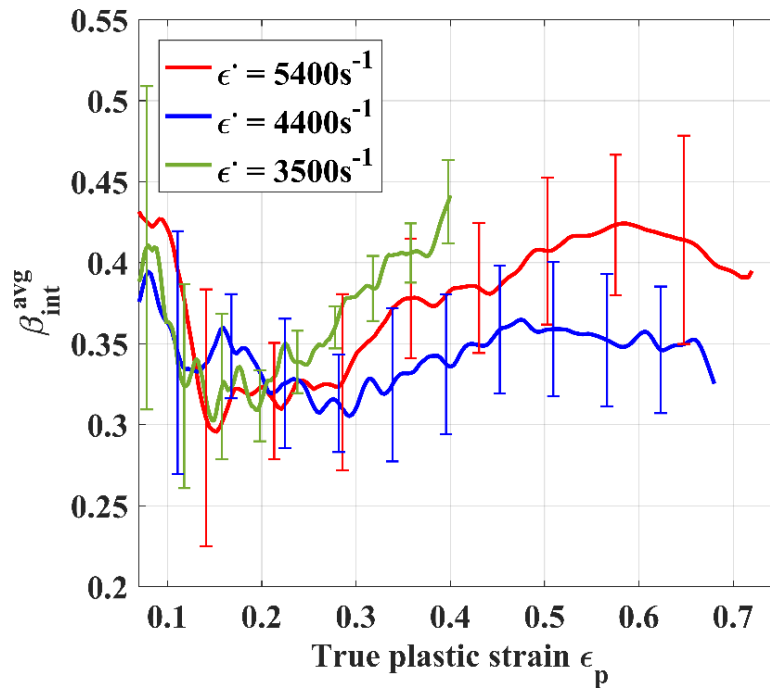


Figure 4-4. Averaged experimental fraction of plastic work converted into heat during deformation. One curve with standard error bars per each strain rate is shown.

The stored energy was further calculated analytically, through Equation 1-4. Figure 4-6 shows a significant difference between the model prediction for the plastic work density (W_P^*) and the strain energy density (E_{stored}) during deformation. A striking observation about the ratio of both quantities can be made; namely, *the former is constantly between three and*

four orders of magnitude greater than the latter. These values, if substituted in Equation 3-10, lead to a calculated Taylor-Quinney coefficient that is practically equal to 1 – in sharp contrast with the experimental results.

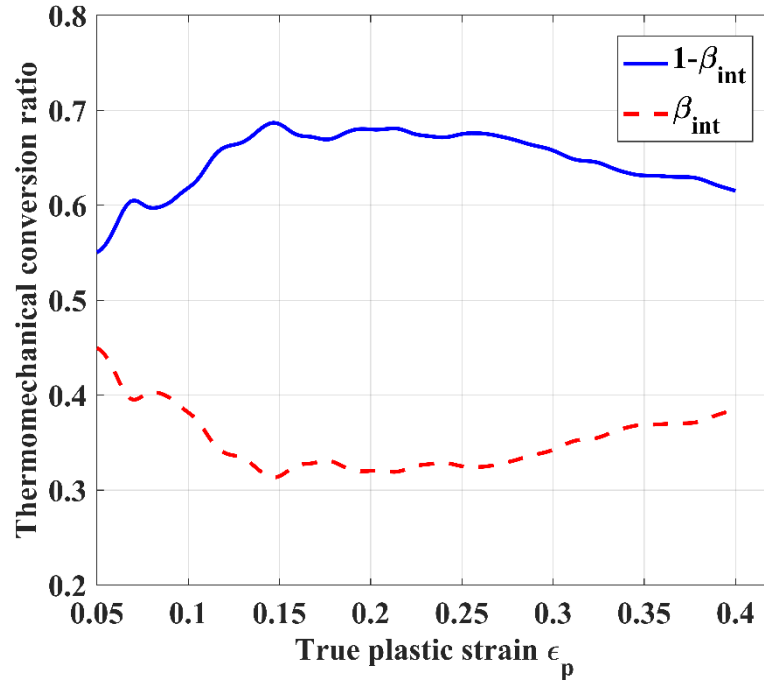


Figure 4-5. Averaged experimental thermomechanical conversion factor (β_{int}) and stored energy fraction evolution on OFHC copper deformed at strain rates of 3500 to 5400 s⁻¹.

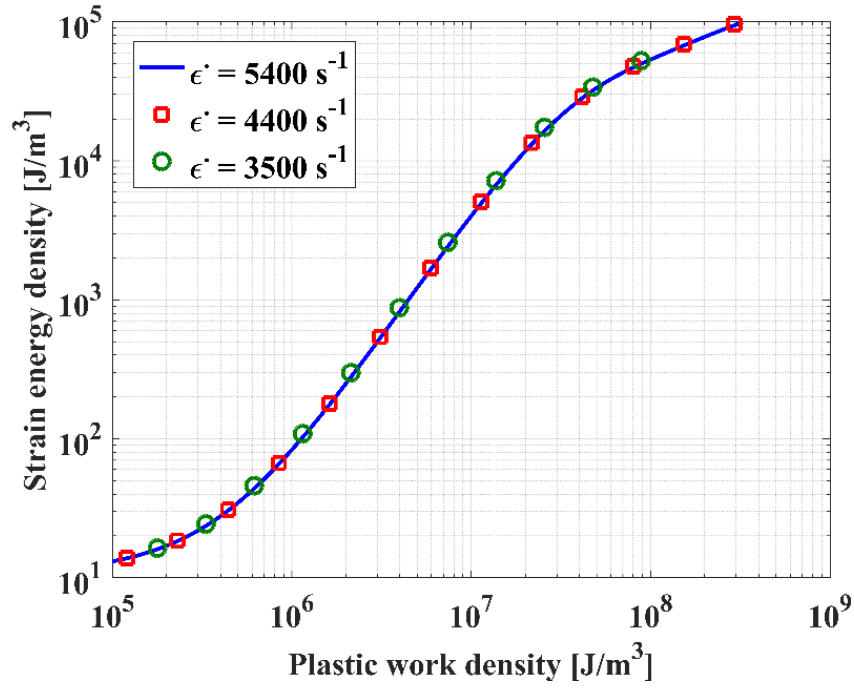


Figure 4-6. Strain energy density vs. Plastic work density. Analytical prediction.

To bring together Equation 1-4 and the experimental observations, we propose the addition of an *ad hoc* factor (Ψ) to the expression, which finally reads:

$$E_{stored} = \Psi \alpha G b^2 \rho_{tot} \quad 4-1$$

where:

$$\Psi = \frac{(1 - \beta_{int}) \int dW_p}{\alpha G b^2 \rho_{tot}} \quad 4-2$$

Since β_{int} is variable with strain and strain rate (Figure 4-4), the factor Ψ will vary accordingly. As a first approximation and for the sake of simplicity, the evolution of Ψ was calculated combining the thermomechanical response of the material under the three specific strain rates used throughout this work. Figure 4-7a presents how Ψ should evolve (solid blue line) with plastic strain to validate the applicability of Equation 1-4 to calculate the stored

energy. The adjusted expression (dashed red line in the same figure) to include in Equation 4-1 was fitted as a linear function as of strains greater than 0.05, due to the variability of the stress-strain curve below that point in the SHPB experiments (see Figure 4-1).

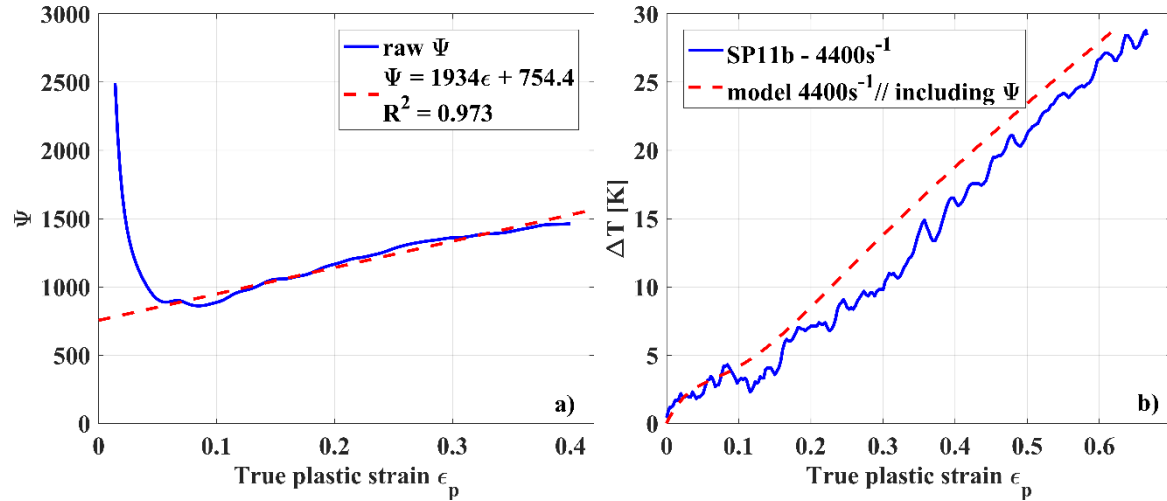


Figure 4-7. a) Evolution of Ψ factor with plastic strain. b) Correction of the increase of temperature during plastic deformation in specimen SP11b, deformed at 4400 s⁻¹.

In Figure 4-7a, a clear trend of increasing Ψ linearly with strain is observed, at least until plastic strains of 0.4 – beyond this point we cannot extrapolate our experimental data. Even so, as shown in Figure 4-7b, the correction of the temperature evolution by using Equation 4-1 in a specimen which deforms plastically up to 0.7 of strain was made, giving satisfactory results on the estimation of the increase of temperature – please refer to Figure 4-3b for a comparison with the model prediction before correction. From the evolution of Ψ that was needed for the experimental results and those obtained from the calculation to match, we suggest that the problem with Equation 1-4 is not simply a missing pre-factor, but rather that some essential element is missing in the formulation.

5. Discussion

As mentioned in the literature review, no data was found on the attempt to calculate analytically the thermomechanical conversion during dynamic deformation with an expression based on the dislocation density in the material – with the exception of the work of Kapoor and Nemat-Nasser (1998). A mismatch similar to the one reported in this paper was found; however, the feasibility of Equation 1-4 in such purpose was not questioned in (Kapoor and Nemat-Nasser, 1998). An initial objective of our work was to modify an existing dislocation-based constitutive model, introducing reasonable corrections based on physical assumptions and experimental work.

Figure 4-1 showed the experimental stress-strain response of as-received OFHC copper deformed at room temperature under different strain rates, which are in good agreement with previous results of other authors, *e.g.* the work of Nemat-Nasser and Li (1998) or Rittel et al. (2012). The model prediction (reported in the same figure) reproduces satisfactorily the work hardening behavior of the material after strains of 0.1, exhibiting on the contrary a poor correlation at very low strains – conceivably due to the inaccuracy of SHPB tests near the elastic vicinity part of the curve (Rittel, 1999). Nonetheless, whether the model totally captures the stress-strain response of the material or not, this is not a drawback concerning the matter addressed here; the model represents a useful analytical tool which opens the way for using Equation 1-4 for the calculation of the strain energy. Accordingly, a dramatic difference regarding the increase of temperature during deformation between the analytical solution and the experimental one was observed (see Figure 4-3b), suggesting that the total dislocation density and/or the strain energy are not accurately calculated. On the other hand,

the ETMB model has demonstrated so far being a reliable approach to define the macroscopic mechanical behavior of ductile materials based on a microscopic (dislocation scale) point of view.

The observed strain rate sensitivity of the material, also captured by the model, may be explained if one analyzes the annihilation terms for both the cell walls and cell interiors, Equations 3-3 and 3-6 respectively. The recovery terms diminish as strain rate increases, resulting in more and more dislocations accumulating in the cells, acting as barriers to the movement of other dislocations and increasing therefore the shear resistance of the cells. The harder phase in the considered two-composite material might be the cell wall, where the density of dislocations should be consistently greater than the one of the softer phase, the cell interior (Estrin et al., 1998; Toth et al., 2002) – as shown in Figure 4-2. The lowering of the dislocation density growth, observed in the previous figure, may be explained by the fact that once the dislocation densities are large enough to trigger recovery, the annihilation rate in both phases increases thus reducing the number of dislocations in the material. The strain rate sensitivity of copper, within a range of different micro- and nano-grain sized compression specimens, was also observed in (Khan et al., 2008).

The second relevant issue was to calculate experimentally the fraction of mechanical work converted into heat during dynamic plastic deformation and compare it to the analytical prediction. It should be noted that the measured temperature rise for all the tested specimens was consistently below the characteristic one of the thermally activated mechanisms for dynamic recovery, *i.e.* climb, strengthening the assumption of considering cross-slip as the annihilation phenomenon for both the cell walls and the cell interiors – confer Section 3. Our

experimental results further support the idea that the stored energy of cold work under adiabatic conditions is greater than the widely-held belief of 0-10% (refer to Figure 4-5); it appears that roughly between 60-70% of the energy spent in plastic deformation remains stored in the material, essentially as microstructural defects – values slightly higher than the previously reported of 30-50% in (Rittel et al., 2012) for the same material. Several authors suggested that the SECW might be the driving force for dynamic recrystallization (DRX), phenomenon that may trigger the formation of adiabatic shear bands (ASB) and the consequent failure of the material (Bacca et al., 2015; Mourad et al., 2017; Rittel et al., 2008).

At that stage, noting the large discrepancy between the analytical and the experimental estimations of the stored energy of cold work for a material whose mechanical response was otherwise adequately described by the modified dislocation-based micromechanical model (Equations 3-3 and 3-6), an *ad hoc* correction factor (Equation 4-2) was introduced into Equation 1-4. It is clear that this *ad hoc* factor Ψ is an *empirical* attempt to remedy the observed discrepancy, **and thus demonstrated the need for a more physical expression**. It is important to note that Benzerga et al. (2005) suggested that although the flow stress and work hardening rate depend mainly on the dislocation density, the stored energy of cold work depends on the details of the dislocation structure that forms, with any long-range dislocation stress field playing a significant role. This might be one possible reason underlying the mentioned inconsistency, and we believe that further research on this should be undertaken.

Further experimental work is required to establish a common pattern for Ψ with several dynamically loaded materials, together with additional analytical work to identify the reasons for the observed discrepancy. **We believe that by studying the discrepancies between the**

measured and calculated values of the stored energy for several materials, common trends may indicate the source of the error in the analytical equation

6. Conclusions

- This study has brought to light an inconsistency between the analytical and the experimental calculations of the thermomechanical conversion during dynamic plastic deformation.
- The analytical solution, based on the energy related to the elastic field around the dislocations and the density of these in the material, appeared to be several orders of magnitude lower than the experimental one – strongly supported, for its part, by the work done in the past years.
- An empirical *ad hoc* correction factor was added to the analytical expression, adjusting the identified mismatch.
- Additional work is required to elucidate the physical reasons underlying the reported discrepancy regarding the calculated stored energy of cold work.

Acknowledgements

The research leading to these results has received funding from the European Union's Horizon2020 Program (Excellent Science, Marie-Sklodowska-Curie Actions) under REA grant agreement 675602 (Project OUTCOME).

Mr. Nieto-Fuentes gratefully acknowledge Mr. Y. Rotbaum, Mr. S. Chen and Mr. L.H. Zhang for their technical support.

The analytical work was supervised by Prof. S. Osovski, while Prof. D. Rittel supervised the experimental part; all authors contributed equally on this paper.

References

- Ashby, M.F., 1970. The deformation of plastically non-homogeneous materials. *Philos. Mag.* 21, 399–424. <https://doi.org/10.1080/14786437008238426>
- Atmani, Z., Haddag, B., Nouari, M., Zenasni, M., 2015. Multi-physics modelling in machining OFHC copper - Coupling of microstructure-based flow stress and grain refinement models. *Procedia CIRP* 31, 545–550. <https://doi.org/10.1016/j.procir.2015.03.023>
- Bacca, M., Hayhurst, D.R., McMeeking, R.M., 2015. Continuous dynamic recrystallization during severe plastic deformation. *Mech. Mater.* 90, 148–156. <https://doi.org/10.1016/j.mechmat.2015.05.008>
- Bacon, D., Hull, D., 2011. Introduction to dislocations, 5th ed, Butterworth-Heinemann. Elsevier. <https://doi.org/10.1017/CBO9781107415324.004>
- Bailey, J.E., Hirsch, P.B., 1960. Dislocation Distribution, Flow Stress, and Stored Energy in Cold-worked Polycrystalline Silver. *Philos. Mag.* 5, 485–497.
- Benzerga, A.A., Bréchet, Y., Needleman, A., Van der Giessen, E., 2005. The stored energy of cold work: Predictions from discrete dislocation plasticity. *Acta Mater.* 53, 4765–4779. <https://doi.org/10.1016/j.actamat.2005.07.011>
- Bever, M.B., Holt, D.L., Titchener, A.L., 1973. The Stored Energy of Cold Work. *Prog. Mater. Sci.* 17, 1–177. [https://doi.org/10.1016/0079-6425\(73\)90001-7](https://doi.org/10.1016/0079-6425(73)90001-7)
- Bjerke, T., Li, Z., Lambros, J., 2002. Role of plasticity in heat generation during high rate deformation and fracture of polycarbonate. *Int. J. Plast.* 18, 549–567. [https://doi.org/10.1016/S0749-6419\(01\)00009-2](https://doi.org/10.1016/S0749-6419(01)00009-2)
- Boley, B.A., Weiner, J.H., 1997. Theory of thermal stresses.
- Cottrell, A.H., 1953. Theory of dislocations. *Prog. Met. Phys.* 4, 205–264. [https://doi.org/10.1016/0502-8205\(53\)90018-5](https://doi.org/10.1016/0502-8205(53)90018-5)
- Ding, H., Shen, N., Shin, Y.C., 2011. Modeling of grain refinement in aluminum and copper subjected to cutting. *Comput. Mater. Sci.* 50, 3016–3025. <https://doi.org/10.1016/j.commatsci.2011.05.020>

- Ding, H., Shin, Y.C., 2011. Dislocation Density-Based Grain Refinement Modeling of Orthogonal Cutting of Commercially Pure Titanium, in: Manufacturing Science and Engineering Conference. pp. 1–10.
- Estrin, Y., Toth, L.S., Bréchet, Y., Kim, H.S., 2006. Modelling of the Evolution of Dislocation Cell Misorientation under Severe Plastic Deformation. *Mater. Sci. Forum* 503–504, 675–680. <https://doi.org/10.4028/www.scientific.net/MSF.503-504.675>
- Estrin, Y., Toth, L.S., Molinari, A., Bréchet, Y., 1998. A dislocation-based model for all hardening stages in large strain deformation. *Acta Mater.* 46, 5509–5522. [https://doi.org/10.1016/s1359-6454\(98\)00196-7](https://doi.org/10.1016/s1359-6454(98)00196-7)
- Galindo-Nava, E.I., Rivera-Díaz-Del-Castillo, P.E.J., 2012. A thermodynamic theory for dislocation cell formation and misorientation in metals. *Acta Mater.* 60, 4370–4378. <https://doi.org/10.1016/j.actamat.2012.05.003>
- Gao, H., Huang, Y., 2003. Geometrically necessary dislocation and size-dependent plasticity. *Scr. Mater.* 48, 113–118. [https://doi.org/10.1016/S1359-6462\(02\)00329-9](https://doi.org/10.1016/S1359-6462(02)00329-9)
- Ghosh, D., Kingstedt, O.T., Ravichandran, G., 2017. Plastic Work to Heat Conversion During High-Strain Rate Deformation of Mg and Mg Alloy. *Metall. Mater. Trans. A Phys. Metall. Mater. Sci.* 48, 14–19. <https://doi.org/10.1007/s11661-016-3825-8>
- Gil Sevillano, J., van Houtte, P., Aernoudt, E., 1980. Large strain work hardening and textures. *Prog. Mater. Sci.* 25, 69–134. [https://doi.org/10.1016/0079-6425\(80\)90001-8](https://doi.org/10.1016/0079-6425(80)90001-8)
- Hirth, J.P., Lothe, J., 1982. *Theory of Dislocations*, 2nd ed. Krieger Publishing Company.
- Hodowany, J., Ravichandran, G., Rosakis, A.J., Rosakis, P., 2000. Partition of plastic work into heat and stored energy in metals. *Exp. Mech.* 40, 113–123. <https://doi.org/10.1007/BF02325036>
- Holt, D.L., 1970. Dislocation Cell Formation in Metals. *J. Appl. Phys.* 41, 3197–3201.
- Huang, M., Rivera-Díaz-del-Castillo, P.E.J., Bouaziz, O., van der Zwaag, S., 2009. A constitutive model for high strain rate deformation in FCC metals based on irreversible thermodynamics. *Mech. Mater.* 41, 982–988. <https://doi.org/10.1016/j.mechmat.2009.05.007>
- Kapoor, R., Nemat-Nasser, S., 1998. Determination of temperature rise during high strain rate deformation. *Mech. Mater.* 27, 1–12. [https://doi.org/10.1016/S0167-6636\(97\)00036-7](https://doi.org/10.1016/S0167-6636(97)00036-7)
- Khan, A.S., Farrokh, B., Takacs, L., 2008. Compressive properties of Cu with different grain sizes: sub-micron to nanometer realm. *J. Mater. Sci.* 43, 3305–3313. <https://doi.org/10.1007/s10853-008-2508-2>
- Khan, A.S., Suh, Y.S., Kazmi, R., 2004. Quasi-static and dynamic loading responses and constitutive modeling of titanium alloys. *Int. J. Plast.* 20, 2233–2248. <https://doi.org/10.1016/j.ijplas.2003.06.005>
- Kocks, U.F., 1970. The relation between polycrystal deformation and single-crystal deformation. *Metall. Mater. Trans. B* 1, 1121–1143. <https://doi.org/10.1007/BF02900224>
- Kocks, U.F., Mecking, H., 2003. Physics and phenomenology of strain hardening: The FCC case. *Prog. Mater. Sci.* 48, 171–273. [https://doi.org/10.1016/S0079-6425\(02\)00003-8](https://doi.org/10.1016/S0079-6425(02)00003-8)
- Kolsky, H., 1949. *An Investigation of the Mechanical Properties of Materials at very High Rates of*

- Loading. Proc. Phys. Soc. Sect. B 62, 676–700. <https://doi.org/10.1088/0370-1301/62/11/302>
- Kuhlmann-Wilsdorf, D., 1989. Theory of plastic deformation: - properties of low energy dislocation structures. Mater. Sci. Eng. A 113, 1–41. [https://doi.org/10.1016/0921-5093\(89\)90290-6](https://doi.org/10.1016/0921-5093(89)90290-6)
- Landau, P., Shneck, R.Z., Makov, G., Venkert, A., 2009. Evolution of dislocation patterns in fcc metals. IOP Conf. Ser. Mater. Sci. Eng. 3. <https://doi.org/10.1088/1757-899X/3/1/012004>
- Lapovok, R., Dalla-Torre, F.H., Sandlin, J., Davies, C.H.J., Pereloma, E. V., Thomson, P.F., Estrin, Y., 2005. Gradient plasticity constitutive model reflecting the ultrafine micro-structure scale: The case of severely deformed copper. J. Mech. Phys. Solids 53, 729–747. <https://doi.org/10.1016/j.jmps.2004.11.006>
- Lemiale, V., Estrin, Y., Kim, H.S., O'Donnell, R., 2011. Forming nanocrystalline structures in metal particle impact. Metall. Mater. Trans. A Phys. Metall. Mater. Sci. 42, 3006–3012. <https://doi.org/10.1007/s11661-010-0588-5>
- Lemiale, V., Estrin, Y., Kim, H.S., O'Donnell, R., 2010. Grain refinement under high strain rate impact: A numerical approach. Comput. Mater. Sci. 48, 124–132. <https://doi.org/10.1016/j.commatsci.2009.12.018>
- Liu, F., Yuan, H., Yin, J., Wang, J.T., 2016. Influence of stacking fault energy and temperature on microstructures and mechanical properties of fcc pure metals processed by equal-channel angular pressing. Mater. Sci. Eng. A 662, 578–587. <https://doi.org/10.1016/j.msea.2016.03.022>
- Ma, W., Li, X., Dai, L., Ling, Z., 2012. Instability criterion of materials in combined stress states and its application to orthogonal cutting process. Int. J. Plast. 30–31, 18–40. <https://doi.org/10.1016/j.ijplas.2011.09.003>
- Macdougall, D.A.S., Harding, J., 1998. The measurement of specimen surface temperature in high-speed tension and torsion tests. Int. J. Impact Eng. 21, 473–488. [https://doi.org/10.1016/S0734-743X\(98\)00007-4](https://doi.org/10.1016/S0734-743X(98)00007-4)
- Mason, J.J., Rosakis, A.J., Ravichandran, G., 1994. On the strain and strain rate dependence of the fraction of plastic work converted to heat: an experimental study using high speed infrared detectors and the Kolsky bar. Mech. Mater. 17, 135–145. [https://doi.org/10.1016/0167-6636\(94\)90054-X](https://doi.org/10.1016/0167-6636(94)90054-X)
- McAuliffe, C., Waisman, H., 2015. A unified model for metal failure capturing shear banding and fracture. Int. J. Plast. 65, 131–151. <https://doi.org/10.1016/j.ijplas.2014.08.016>
- Mckenzie, P.W.J., Lapovok, R., Estrin, Y., 2007. The influence of back pressure on ECAP processed AA 6016: Modeling and experiment. Acta Mater. 55, 2985–2993. <https://doi.org/10.1016/j.actamat.2006.12.038>
- Meyers, M.A., 1994. Dynamic Behavior of Materials, Dynamic Behavior of Materials. John Wiley & Sons.
- Meyers, M.A., LaSalvia, J.C., Nesterenko, V.F., Chen, Y.J., Kad, B.K., 1997. Dynamic Recrystallization in High Strain Rate Deformation. Third Int. Conf. Recryst. Relat. Phenom. 279–286.
- Mourad, H.M., Bronkhorst, C.A., Livescu, V., Plohr, J.N., Cerreta, E.K., 2017. Modeling and simulation framework for dynamic strain localization in elasto-viscoplastic metallic materials

- subject to large deformations. *Int. J. Plast.* 88, 1–26. <https://doi.org/10.1016/j.ijplas.2016.09.009>
- Mughrabi, H., 1987. A two-parameter description of heterogeneous dislocation distributions in deformed metal crystals. *Mater. Sci. Eng.* 85, 15–31. [https://doi.org/10.1016/0025-5416\(87\)90463-0](https://doi.org/10.1016/0025-5416(87)90463-0)
- Nabarro, F.R.N., Basinski, Z.S., Holt, D.B., 1964. The Plasticity of Single Crystals. *Adv. Phys.* 13, 193–323. <https://doi.org/10.1080/00018736400101031>
- Needleman, A., Sevillano, J.G., 2003. Preface to the viewpoint set on: Geometrically necessary dislocations and size dependent plasticity. *Scr. Mater.* 48, 109–111. [https://doi.org/10.1016/S1359-6462\(02\)00336-6](https://doi.org/10.1016/S1359-6462(02)00336-6)
- Nemat-Nasser, S., Li, Y., 1998. Flow stress of F.C.C. polycrystals with application to OFHC Cu. *Acta Mater.* 46, 565–577. [https://doi.org/10.1016/S1359-6454\(97\)00230-9](https://doi.org/10.1016/S1359-6454(97)00230-9)
- Nes, E., 1998. Modelling of work hardening and stress saturation in FCC metals. *Prog. Mater. Sci.* 41, 129–193. [https://doi.org/10.1016/S0079-6425\(97\)00032-7](https://doi.org/10.1016/S0079-6425(97)00032-7)
- Nye, J.F., 1953. Some Geometrical Relations in Dislocated Crystals. *Acta Metall.* 1, 153–162.
- Parvin, H., Kazeminezhad, M., 2014. Development a dislocation density based model considering the effect of stacking fault energy: Severe plastic deformation. *Comput. Mater. Sci.* 95, 250–255. <https://doi.org/10.1016/j.commatsci.2014.07.027>
- Rittel, D., 1999. On the conversion of plastic work to heat during high strain rate deformation of glassy polymers. *Mech. Mater.* 31, 131–139. [https://doi.org/10.1016/S0167-6636\(98\)00063-5](https://doi.org/10.1016/S0167-6636(98)00063-5)
- Rittel, D., Bhattacharyya, A., Poon, B., Zhao, J., Ravichandran, G., 2007. Thermomechanical characterization of pure polycrystalline tantalum. *Mater. Sci. Eng. A* 447, 65–70. <https://doi.org/10.1016/j.msea.2006.10.064>
- Rittel, D., Kidane, A.A., Alkhader, M., Venkert, A., Landau, P., Ravichandran, G., 2012. On the dynamically stored energy of cold work in pure single crystal and polycrystalline copper. *Acta Mater.* 60, 3719–3728. <https://doi.org/10.1016/j.actamat.2012.03.029>
- Rittel, D., Landau, P., Venkert, A., 2008. Dynamic Recrystallization as a Potential Cause for Adiabatic Shear Failure. *Phys. Rev. Lett.* 101. <https://doi.org/10.1103/PhysRevLett.101.165501>
- Rittel, D., Osovski, S., 2010. Dynamic failure by adiabatic shear banding. *Int. J. Fract.* 162, 177–185. <https://doi.org/10.1007/s10704-010-9475-8>
- Rittel, D., Rabin, Y., 2000. An investigation of the heat generated during cyclic loading of two glassy polymers. Part II: Thermal analysis. *Mech. Mater.* 32, 149–159. [https://doi.org/10.1016/S0167-6636\(99\)00052-6](https://doi.org/10.1016/S0167-6636(99)00052-6)
- Rittel, D., Silva, M.L., Poon, B., Ravichandran, G., 2009. Thermomechanical behavior of single crystalline tantalum in the static and dynamic regime. *Mech. Mater.* 41, 1323–1329. <https://doi.org/10.1016/j.mechmat.2009.08.001>
- Rittel, D., Wang, Z.G., 2008. Thermo-mechanical aspects of adiabatic shear failure of AM50 and Ti6Al4V alloys. *Mech. Mater.* 40, 629–635. <https://doi.org/10.1016/j.mechmat.2008.03.002>
- Rittel, D., Zhang, L.H., Osovski, S., 2017. The dependence of the Taylor–Quinney coefficient on the dynamic loading mode. *J. Mech. Phys. Solids* 107, 96–114.

<https://doi.org/10.1016/j.jmps.2017.06.016>

- Rollett, A.D., Kocks, U.F., 1993. A Review of the Stages of Work Hardening. *Solid State Phenom.* 35–36, 1–18. <https://doi.org/10.4028/www.scientific.net/SSP.35-36.1>
- Simon, N.J., Drexler, E.S., Reed, R.P., 1992. Properties of copper and copper alloys at cryogenic temperatures, National Institute of Standards and Technology (NIST). National Institute of Standards and Technology, Gaithersburg, MD. <https://doi.org/10.6028/NIST.MONO.177>
- Taylor, G.I., 1934. The Mechanism of Plastic Deformation of Crystals. *Proc. R. Soc. London* 145, 362–387. <https://doi.org/10.1098/rspa.1983.0054>
- Toth, L.S., Molinari, A., Estrin, Y., 2002. Strain Hardening at Large Strains as Predicted by Dislocation Based Polycrystal Plasticity Model. *J. Eng. Mater. Technol.* 124, 71. <https://doi.org/10.1115/1.1421350>
- Wu, X.X., San, X.Y., Liang, X.G., Gong, Y.L., Zhu, X.K., 2013. Effect of stacking fault energy on mechanical behavior of cold-forging Cu and Cu alloys. *Mater. Des.* 47, 372–376. <https://doi.org/10.1016/j.matdes.2012.12.006>
- Zerilli, F.J., Armstrong, R.W., 1987. Dislocation mechanics based constitutive relations for material dynamics calculations. *J. Appl. Phys.* 61, 1816–1825. <https://doi.org/10.1063/1.338024>
- Zhang, Z., Eakins, D.E., Dunne, F.P.E., 2016. On the formation of adiabatic shear bands in textured HCP polycrystals. *Int. J. Plast.* 79, 196–216. <https://doi.org/10.1016/j.ijplas.2015.12.004>

Appendix A

The evolution of the density of GNDs with strain for the two-dimensional case can be calculated as (Estrin et al., 2006):

$$\left(\frac{d\rho_{GND}}{d\gamma} \right) = \xi \frac{4\beta^* \sqrt{1-f}}{bdf} \quad 0-1$$

where ξ can be calculated as (Rittel and Osovski, 2010):

$$\xi = \xi_0 \exp\left(-\frac{\theta}{\theta_0}\right) \quad A-2$$

being ξ_0 an initial value for the volume fraction of GNDs in the walls, θ_0 the decay rate of increase of GNDs, and θ the misorientation angle between adjacent cells, whose evolution can be predicted as (Estrin et al., 2006):

$$\frac{d\theta}{d\gamma} = 2\beta^* \xi \frac{1}{\theta} \frac{b\sqrt{1-f}}{df} \quad \text{A-3}$$

In order to estimate the evolution of the new formed dislocation cell d let us now look at the selection of the proportionality coefficient, K , a parameter that critically affects the evolution of the cell size. Lapovok et al. (2005) reported that the dependence of K on the accumulated plastic strain can be expressed by:

$$K = K_0 + K_1 \exp(-\gamma / \kappa) \quad \text{A-4}$$

where the parameters K_0 , K_1 and κ are used to fit the cell size evolution at different levels of strain. Even though the introduction of new parameters may result in additional experimental work, the flexibility of the model would increase substantially. Here we adopt the expression for K_0 developed by Galindo-Nava and Rivera-Díaz-Del-Castillo (2012) based on material dependent parameters, an approach followed by Liu et al. (2016):

$$K_0 = \frac{24\pi(1-\nu)}{(2+\nu)} \left(\frac{1}{2} + \frac{T\Delta S}{Gb^3} \right) \quad \text{A-5}$$

where ν is Poisson's coefficient, T is the deformation temperature, and ΔS is the statistical entropy, which can be calculated as:

$$\Delta S = k \ln \left(\frac{bc\rho_m + \mathcal{G}}{\dot{\gamma}} \right) \quad \text{A-6}$$

being k the Boltzmann constant, c the speed of sound in the material, ρ_m the mobile dislocation line density, and $\mathcal{G}$ the vacancy jump frequency, expressed as:

$$\mathcal{G} = \mathcal{G}_D \exp\left(\frac{-E_m}{RT}\right) \quad \text{A-7}$$

where E_m is the vacancy migration energy, and R is the ideal gas constant.