Latent Heat Saturation in Microstructural Evolution by Severe Plastic Deformation

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Abstract

During plastic deformation, most of the dissipated work is released as heat, but a fraction of it, usually small, is stored in the microstructure, is called *latent heat* and is associated with the network of dislocations that develops. The rate of energy storage in the microstructure divided by the rate of plastic dissipation is defined as the *latent heat capacity*. Latent heat remains stored in the microstructure of cold worked specimens after quenching. This energy is associated with modified mechanical properties, *e.g.* hardness, and is released upon annealing. Saturation of this stored energy has been observed in experiments after a specific amount of plastic deformation is reached. A thermodynamically consistent model for continuous dynamic recrystallization is proposed in this paper with the aim of explaining the phenomenon of latent heat saturation and relating it to grain refinement. The proposed model has three essential features: (i) the latent heat increases in the specimen during plastic deformation as plastic work is continuously dissipated; (ii) the rate of latent heat storage per unit work, *i.e.* the latent heat capacity, is related to the internal architecture of the microstructure and decreases to zero as a consequence of microstructural evolution; (iii) the relationship between the latent heat and the microstructure is described through the use of two parameters: (a) the dislocation density and (b) the average grain diameter. A comparison of the proposed model with experiments is reported and a validation for the prediction of microstructural evolution, as well as the evolution of the latent heat and latent heat capacity, is provided.

Keywords: Microstructural evolution; Latent heat; Reverse Hall-Petch effect; Recrystallization.

1. Introduction

The mechanical properties of a material depend on its physical state, and in particular, for solid materials, on the configuration of the microstructure. Many authors have developed constitutive models that are sensitive to the heterogeneity of the material, as well as its microstructure, for

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small deformations (Mindlin 1964, Bacca *et al.* 2013) and for large deformations (Aifantis 1984). Less attention has been dedicated to the development of constitutive models that are sensitive to the evolution of the microstructure, as well as the mechanical properties linked to it. The proposed work attempts to contribute to this field on a thermodynamically consistent basis.

Microstructural evolution occurs via mechanical processes that involve cold working of the material. The resulting change in microstructure is associated with the amount of plastic deformation experienced by the material and becomes significant after severe plastic deformation (SPD) associated with processes such as low-speed machining (Shankar *et al.* 2005, Bacca, Hayhurst and McMeeking 2015). Experiments performed by Taylor and Quinney (1934) on torsion of metal rods have shown how this evolution is measured by *latent heat*, *i.e.* the energy that remains stored in the specimen after the specimen is quenched. This energy is considered to be stored in the microstructure, is responsible for the evolution of the microstructure as it is associated with the network of dislocations that develops, and increases continuously with plastic work (Bever, Holt and Titchener 1973). The Taylor and Quinney (1934) experiments on torsion, as well as experiments on machining (Saldana, King and Chandrasekar 2012) demonstrate saturation of the latent heat for a finite amount of plastic strain, with continuous reduction to zero of the rate of storage of latent heat per unit work (called the *latent heat capacity*).

Some constitutive models based on latent heat storage have previously been developed with the aim of predicting microstructure evolution in metals (Bernacki *et al.* 2009, Le and Kochmann 2009, Quan *et al.* 2011, Brown and Bammann 2012, Bacca *et al.* 2015), with a focus on the phenomenon of dynamic recrystallization. This phenomenon has also been studied with different approaches such as phase field models (Militzer 2011, Moelans *et al.* 2013, Sreekala and Haataja 2007, Suwa, Saito and Onodera 2008), which considers the nucleation and subsequent growth of new grains within the “old” microstructure, and with the use of finite element techniques as well as other methodologies such as cellular automata (Hallberg 2011). However, the *latent heat saturation* (LHS) phenomenon is neglected in those models and a physical interpretation has not been reported in the literature.

In the present paper, a thermodynamically consistent model for continuous dynamic recrystallization (CDRX) created by SPD is provided. In this model, an evolution of the micro and nanomechanisms that accommodate macroscopic plastic deformation is considered, and a physical interpretation for the phenomenon of LHS is provided.

As will be explained in this paper, grain refinement is created by CDRX and gives a reduction of the average grain diameter, allowing the microstructure ultimately to develop a grain boundary sliding (GBS) mechanism for plastic deformation. When this mechanism of plastic deformation becomes predominant over other mechanisms associated with dislocation motion, microstructure evolution is complete and no further energy can be stored in the system as latent heat, giving LHS.

An explanation of the proposed model and all its features is provided in Section 2; results on the prediction of the evolution of the microstructure as well as the latent heat and latent heat capacity

are given in Section 3; discussion of the model and its conditions of applicability are reported in Section 4; finally some conclusions are drawn in Section 5.

2. The constitutive model

2.1 Basic principles

In the present work, an improved version of the simple model for CDRX developed by Bacca *et al.* (2015) is developed. The basic principles of the original model are explained in this section, with more detail given in Bacca *et al.* (2015), while the proposed new features are explained in the subsequent sections.

In the model the yield strength is given by superposition of two main contributions: (i) Dislocation strengthening, which mechanism involves pinning of dislocations by others, as described by Taylor (1934); (ii) Grain boundary strengthening, as described by Hall (1951) and Petch (1953). The total yield strength in shear, in agreement with Castro-Fernandez and Sellars (1989) and Le and Kochmann (2009), has the form

$$\tau_y = \alpha b \mu \sqrt{\rho} + \lambda \left(\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d_0}} \right), \quad (1)$$

where α is a phenomenological constant for Taylor hardening (usually taken as unity), b is the Burgers vector, μ is the shear modulus, ρ is the dislocation density, λ is the Hall-Petch coefficient, d is the current average grain size, and d_0 is a reference grain size that is sufficiently large so that the Hall-Petch effect is negligible. With condition $d = d_0$, eq. (1) only accounts for changes to hardness caused by changes to ρ .

During plastic deformation, energy conservation can be written neglecting reversibly stored macroscopic elastic strain energy, *i.e.* identifying only dissipative terms, in order to obtain the rate equation (with superposed dots indicating differentiation with respect to time or rates)

$$\tau_y \dot{\gamma}_p = \dot{Q} + \dot{U}_m, \quad (2)$$

where $\dot{\gamma}_p$ is the rate of change of the shear equivalent plastic strain, $\dot{Q}$ is the rate per unit volume at which mechanical work is dissipated as heat, and $\dot{U}_m$ is the rate per unit volume at which plastic work is stored in the microstructure as latent heat (the *latent heat rate*) (Taylor and Quinney 1934). The right-hand side of eq. (2) corresponds to the amount of plastic work per unit volume supplied to the system at the unit time and can be associated with the rate of change of a hardening energy potential W_p , for which $\tau_y = \partial W_p / \partial \gamma_p$, thus $\dot{W}_p = \tau_y \dot{\gamma}_p$ (Chang and Kochmann 2015). The left-hand side of eq. (2) is the rate per unit volume at which the applied loads do plastic work on the material. If we define a latent heat capacity, κ , as the rate at which plastic work is stored in the microstructure as latent heat, divided by the rate of total plastic work, we have

$$\dot{U}_m = \kappa \tau_y \dot{\gamma}_p. \quad (3)$$

As will be explained in section 2.3 κ tends to reduce for continued plastic strain.

Experimental measurement of energy storage and dissipation have been carried out mostly through observations of the *Taylor and Quinney* (T&Q) *coefficient*, β , which determines the rate at which plastic work is dissipated as heat divided by the rate of total plastic work, giving

$$\dot{Q} = \beta \tau_y \dot{\gamma}_p. \quad (4)$$

Eq. (3) and eq. (4) can be substituted into eq. (2) to give

$$\kappa = 1 - \beta. \quad (5)$$

The microstructural energy U_m , also known as the latent heat, is assumed to be as described by Berdichevsky (2006), which is given by the sum of two contributions due to dislocation density, ρ , and grain size, d , respectively, such that

$$U_m(\rho, d) = -k\mu \left[\text{Log} \left(1 - \sqrt{\frac{\rho}{\rho_s}} \right) + \sqrt{\frac{\rho}{\rho_s}} \right] + \frac{\chi \Gamma_s}{2d}, \quad (6)$$

where k is a constant, χ is a grain shape factor (its value is 3 if we consider spherical grains), Γ_s is the average interface energy of the grain boundaries, and ρ_s is a theoretical saturation limit for the dislocation density, *i.e.* in the absence of recrystallization ρ_s is the maximum dislocation storage capacity, for which the latent heat becomes indefinitely large (Berdichevsky 2006). The constant k is defined by $k\mu = \kappa_0 \tau_s \gamma_0$ (Bacca *et al.* 2015), where κ_0 is the initial latent heat capacity (associated with zero plastic strain), and τ_s and γ_0 are parameters that will be defined later in this section.

Differentiation of eq. (6) and substitution of the result into eq. (3), gives

$$\frac{k\mu \dot{\rho}}{2\rho_s \left(1 - \sqrt{\rho / \rho_s} \right)} - \frac{\chi \Gamma_s}{2d^2} \dot{d} = \kappa \tau_y \dot{\gamma}_p, \quad (7)$$

which is a differential equation that relates the microstructural parameters ρ and d to the shear equivalent plastic strain γ_p .

As many theories and experiments indicate, CDRX commences only after a critical amount of plastic deformation is reached, associated with instability in the intragranular dislocation structure (Bailey and Hirsch 1962, Luton and Sellars 1969, Roberts and Ahlblom 1978, [Quan *et al.* 2011](#)). This instability leads to the creation of low angle subgrain boundaries condensed from

existing dislocations in the microstructure. At this point, CDRX has started and all existing dislocations and many of the new ones produced will eventually be adsorbed into the subgrain boundaries, causing increasing misorientation across them until new, distinct, refined grains are created.

From the above observations, microstructural evolution is divided into two main stages (Le and Kochmann 2009, Bacca *et al.* 2015): *prior to recrystallization*, and *during recrystallization*. The first stage is summarized by the conditions $\dot{d} = 0$, $d = d_0$, as no grain refinement occurs at this stage, and $\kappa = \kappa_0$, which implies that κ can evolve only during CDRX.

These conditions allow us to integrate eq. (7) and obtain a relationship between γ_p and ρ . From this, a relationship between γ_p and τ_y is obtained by using eq. (1) and has the form of the Voce law (Voce 1948)

$$\tau_y = \tau_0 + (\tau_s - \tau_0) \left[1 - \exp(-\gamma_p / \gamma_0) \right], \quad (8)$$

valid for $\gamma_p \leq \gamma_c$, where γ_c is the critical amount of plastic strain for initiation of CDRX. The parameter τ_0 is the initial yield strength in shear, τ_s introduced above in connection with eq. (6) is given by $\tau_s = \alpha b \mu \sqrt{\rho_s}$, is the theoretical maximum value of τ_y that can be reached if no recrystallization occurs and is associated with the maximum dislocation density ρ_s that can be stored by the microstructure, and γ_0 is a representative shear strain, also introduced above. The parameters γ_0 and τ_s are influenced by strain rate and temperature as measured by Kocks (1976). We take implicit account of this influence, as the material parameters used in the model are calibrated to the evolution of hardness for continued plastic strain at constant strain rate and temperature. The dislocation density ρ in this stage is obtained from eq. (1), giving $\rho_0 = (\tau_0 / \alpha b \mu)^2$ as the initial dislocation density. The relationship between yield strength and plastic strain included in eq. (8) is empirical as it arises from experimental observations. It has been used by Berdichevsky (2006) to formulate the first term on the right hand side of eq. (6) so it unsurprisingly generates eq. (8) when grain size is constrained to be d_0 and eq. (7) is integrated.

When CDRX starts, we adopt the condition of steady state yield strength as experiments do not evidence significant strain hardening or softening during this process (Le and Kochmann 2009). Thus

$$\tau_y = \tau_c, \quad \dot{\tau}_y = 0, \quad (9)$$

where τ_c is obtained from eq. (8) for $\gamma_p = \gamma_c$, and corresponds to the critical yield strength in shear when recrystallization starts. Substituting eq. (1) into eq. (9) and the result into eq. (7), we have

$$\left[\frac{\lambda k \sqrt{\rho(d)}}{2\alpha b \rho_s d^{3/2} \left(1 - \sqrt{\rho(d)/\rho_s}\right)} - \frac{\chi \Gamma_s}{2d^2} \right] \dot{d} = \kappa \tau_c \dot{\gamma}_p, \quad (10)$$

with

$$\sqrt{\rho(d)} = \frac{1}{\alpha b \mu} \left[\tau_c - \lambda \left(\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d_0}} \right) \right]. \quad (11)$$

The results in eq. (10) and (11), with the hypothesis of constant latent heat capacity $\kappa = \kappa_0$, have been integrated by Bacca *et al.* (2015) to obtain qualitative matching with experiments on machining. The hypothesis of $\kappa = \kappa_0$ gives indefinite increase of the latent heat during continued plastic strain, in disagreement with experiments, and leads to an underestimation of the grain size for large plastic deformations. The proposed, modified model, as will be explained in the next sections, considers a microstructure dependent latent heat capacity in order to overcome the aforementioned limitations and to give better agreement with experiments.

2.2 Grain boundary sliding mechanism

Macroscopic plastic deformation is accommodated through deformation mechanisms at the micro and nanoscale. In the proposed, modified model, two main mechanisms are identified as responsible for plastic deformation: (i) dislocation motion (mainly dislocation glide) (DM) and (ii) grain boundary sliding (GBS). The plastic strain rate is described as the superposition of the strain rate generated by each single mechanism, as proposed by Langdon (1994), giving, for the shear component, the condition

$$\dot{\gamma}_p = \dot{\gamma}_{DM} + \dot{\gamma}_{GBS}. \quad (12)$$

A phenomenological formulation that describes both terms on the right-hand side of eq. (12), for high temperature creep and superplasticity, has been proposed by Langdon (1994) as

$$\dot{\gamma}_i = \frac{A_i D_i \mu b}{\bar{k} T} \left(\frac{b}{d} \right)^{p_i} \left(\frac{\tau_y}{\mu} \right)^{n_i}, \quad i = DM, GBS, \quad (13)$$

where $\bar{k}$ is the Boltzmann constant, T is the temperature, D_i is the appropriate diffusion coefficient, A_i , p_i and n_i are positive constants calibrated from experiments. The result in eq. (13) reveals the influence of grain size d on GBS activity through b/d , the ratio of the average size b

of the core of a gliding dislocation to the average size d of a sliding grain (Rachinger 1952-53). The exponents on the grain size term in eq. (13) are deduced to be $p_{DM} = 0$, and $p_{GBS} = 1$ for most experiments (Langdon 1994). Earlier work by Raj and Ashby (1971) provided a similar model to describe GBS with $p_{GBS} = 2$ and proved its validity also at low temperature and small grain size. We observe negligible discrepancy in the results of our model for p_{GBS} that ranges from 1 to 2; thus we have chosen $p_{GBS} = 1$. Given the adopted values for p_{DM} and p_{GBS} , increasing GBS activity is observed as grains become smaller while DM activity remains independent of the grain size. The latter observation suggests a limitation on the validity of eq. (13) when grain refinement from CDRX is involved; *i.e.* dislocation adsorption caused by recrystallization should diminish DM activity. This leads to an implicit dependence of the DM strain rate contribution on the grain size d , a dependence not captured by Langdon's model. To overcome this limitation, we take both $\dot{\gamma}_{DM}$ and $\dot{\gamma}_{GBS}$ to be grain size dependent, with only the latter one described by eq.(13), so that the fractions they contribute to the total strain rate change as the grain size diminishes, with the GBS fraction rising (according to eq. (13)) and the DM one falling.

When the grain size reaches the nanoscale, experiments show a mismatch with respect to the Hall-Petch law, as expressed in the second term on the right-hand side of eq. (1). In this regime GBS substitutes for DM as the primary deformation mechanism, and it is observed that the yield strength diminishes with a reduction in grain size (Chokshi *et al.* 1989). This reverse Hall-Petch effect arises because the energy barrier to GBS is less in microstructures with smaller grains as less geometric distortion is needed to accommodate the resulting plastic flow. Experiments indicate a critical grain size d_c at which the transition between the Hall-Petch effect and its reverse occurs (Chokshi *et al.* 1989). This critical grain size is influenced by the temperature, for the aluminum alloy Al6061-T6 at room temperature this grain size is around 100 nm (Maung, Earthman and Mohamed 2012), and at that transition DM ceases. From the latter observation, and the dependence of $\dot{\gamma}_{GBS}$ on d in eq. (13), we deduce the form

$$\dot{\gamma}_{GBS}(d) = \dot{\gamma}_p \frac{d_c}{d}, \quad \dot{\gamma}_{DM}(d) = \dot{\gamma}_p \left(1 - \frac{d_c}{d}\right). \quad (14)$$

where $\dot{\gamma}_p d_c$ summarizes all the constants included in eq. (13) with the exception of d . Thus for $d = d_c$, $\dot{\gamma}_{GBS} = \dot{\gamma}_p$ and $\dot{\gamma}_{DM} = 0$. We now consider $d = d_0$, where d_0 as above is the grain size prior to any refinement, in a situation where $d_c = 100$ nm and $d_0 = 75$ μ m as in the case of experimental data for Al6061-T6 (Shankar *et al.* 2005, Maung *et al.* 2012). In this situation, $\dot{\gamma}_{GBS} \approx 0$, and $\dot{\gamma}_{DM} \approx \dot{\gamma}_p$. This observation shows that DM dominates the strain rate at large grain size prior to refinement, but GBS has taken over entirely if CDRX reduces the grain size to 100 nm, in agreement with the experimental observations.

2.3 Saturation of the latent heat

In eq. (4), the T&Q coefficient β depends on the microstructural configuration (grain size d and dislocation density ρ) as the heat generation mechanism will change as a consequence of

microstructural evolution. Superposition of the strain rates due to GBS and DM in eq. (12) is extended to heat generation in eq. (4) as

$$\dot{Q} = \beta_{\text{DM}} \tau_y \dot{\gamma}_{\text{DM}} + \beta_{\text{GBS}} \tau_y \dot{\gamma}_{\text{GBS}}, \quad (15)$$

where β_{DM} and β_{GBS} are partial T&Q coefficients related to each individual mechanism. We take these to be constant and thus independent of ρ and d . Furthermore, we consider $\beta_{\text{GBS}} = 1$, based on the observation that GBS lacks a mechanism for increasing the energy that is globally stored in the microstructure. This is in contrast to DM where Frank-Read sources multiply dislocations and leave them stored statistically in the microstructure, including their associated elastic strain and dislocation core energies. In most nanocrystalline metals, GBS has been observed to be accompanied by grain boundary rotations (Shan *et al.* 2004), which can increase the boundary misorientation angle and, according to the Read and Shokley (1950) equation, the grain boundary energy Γ_s ¹. This occurs by adsorption of intragranular statistically stored dislocations which then become geometrically necessary to accommodate the increased misorientation of the grain boundary. In such reconfiguration, the energy stored by a single dislocation that transits from the forest to the grain boundary becomes smaller (not greater), therefore there is no global increase of energy U_m associated with GBS.

If we substitute eq. (14) into eq. (15) to calculate β and substitute it into eq. (5), we obtain an expression for the latent heat capacity κ as a function of the average grain size d that, with the initial condition $\kappa(d_0) = \kappa_0$, gives

$$\kappa(d) = \kappa_0 \left(\frac{1 - d_c / d}{1 - d_c / d_0} \right). \quad (16)$$

The result in eq. (16) gives $\kappa = 0$ for $d = d_c$ which implies saturation of the latent heat for a critical grain size. This is in agreement with the hypothesis of negligible DM and the consequent impossibility of storage of energy in the microstructure by the generation of dislocations.

3. Results

3.1 Physical parameters and calibration of the model

Figure 1 reports a schematic representation of the machining experiments of Shankar *et al.* (2005) used for calibration and subsequent validation of the proposed model. The parameters of the experiment are given in Table 1, where we state the cutting speed v_0 , the rake angle ϑ , and the feed a_0 , defined in Figure 1. In this experiment, the total shear equivalent plastic strain γ_p inside the chip is related to the rake angle and has been determined with an empirical relationship through the measurement of the chip thickness. In Table 1 we report three different values of the rake angle and the total plastic strain that is associated with each value. Figure 1 also shows the primary deformation zone (PDZ) where the strain is developed and where the material transits

¹ However we neglect this change as a first approximation.

from its annealed state (in the domain of the “material being removed”) to the cold worked state (inside the chip). A relevant strain rate is observed in the PDZ while outside this domain the strain rate is negligible. In this experiment a low cutting speed is also adopted in order to sustain the hypothesis of negligible temperature rise and allow for the consideration of $T \approx T_r$ (with T_r the room temperature).

Parameter/Measurements	Symbol	Values		
Rake angle	ϑ	20°	-5°	-20°
Cutting speed	v_0	10 mm/s		
Feed	a_0	0.150 mm		
Shear equivalent plastic strain	γ_p	1.7	3.2	5.2
Average grain size after machining	d	150 nm	82 nm	75 nm

Table 1: Parameters and *measurements* for the machining experiment of Shankar *et al.* (2005).

The experiments of Shankar *et al.* (2005) utilize Al6061-T6 specimens. This material is an aluminum alloy, and its physical properties are given in Table 2.

Parameter	Symbol	Value
Shear modulus	μ	25 GPa *
Grain shape factor	χ	3 *
Grain Interface Energy	Γ_s	0.625 J / m ² *
Hall-Petch constant	λ	0.01 MPa m ^{1/2} *
Taylor constant	α	1 **
Burger vector	b	2.86·10 ⁻¹⁰ m ***
Grain size when annealed	d_0	75 μ m ****
Critical grain size for inversion of the Hall-Petch effect	d_c	100 nm *****

Table 2: Material parameters for Al6061-T6. The sources are * Le and Kochmann 2009, ** Taylor 1934, *** Rösler, Harders and Bäker (2007), **** Shankar *et al.* 2005, ***** Maung *et al.* 2012.

In addition to the parameters given in Table 2, the other parameters appearing in eq. (8) through (11) are reported in Table 3. These parameters are obtained from the calibration carried out by Bacca *et al.* (2015) by use of the results of experiments by Shankar *et al.* (2005).

<i>Parameter</i>	<i>Symbol</i>	<i>Value</i>
Initial yield strength in shear	τ_0	186.91 MPa
Yield strength in shear for steady state conditions	τ_c	258.27 MPa
Saturation yield strength in shear	τ_s	1.74 GPa
Initial latent heat capacity	κ_0	12%
Reference shear strain	γ_0	1.04
Critical shear equivalent plastic strain	γ_c	0.005

Table 3: Calibrated parameters for the model based on machining experiments for the aluminum alloy Al6061-T6 (Shankar *et al.* 2005). For details about the calibration see Bacca *et al.* (2015).

As can be observed in Table 3, τ_s is comparable to the theoretical shear strength given by $\mu / 2\pi$. This is due to the phenomenon of saturation of dislocations which gives a microstructure that is such densely populated by defects that the activation energy needed for creating plastic deformation is comparable to the energy needed to deform a perfect crystal.

3.2 Theoretical results and comparison with experiments

Figure 2 shows the mechanical behavior of Al6061-T6 subject to large plastic deformations, for the same strain rate and temperature as in the Shankar *et al.* (2005) machining experiments. For $\gamma_p < \gamma_c$ the behavior is described by eq. (8), whereas for $\gamma_p > \gamma_c$ the mechanical behavior is described by eq. (9) as perfectly plastic. These theoretical values are indicated with a solid line, while the experimental values (taken from Shankar *et al.* 2005) are indicated with open circles and relative error bars. This figure reports the evolution of the Vicker hardness H_v for an increasing plastic strain, as this quantity is associated with the yield strength in shear by the relationship $\tau_y = H_v / 3\sqrt{3}$ (Nurislamova *et al.* 2008). In this comparison, the model has been calibrated by choosing τ_0 and τ_c in order to give minimum discrepancy between the associated H_0 and H_c and all the experimental points (in the range described by the error bars). With the choice reported in Table 3, the deviation of the proposed horizontal line from the limits of the error bars of the experimental data points is on average 0.67% and has a maximum of 2.6%. The error committed in the measurement of the hardness, in the same data points (taking one half of the amplitude of the error bars in Figure 2), is on average 2.13% with a maximum of 3.07%. From this observation it follows that the error committed in the approximation of the hardening behavior with the proposed model is smaller than the error committed in the obtainment of the values of the data points in Figure 2. Therefore the proposed model is considered to be in good agreement with experiments.

The parameters' value reported in Tables 2-3 can be utilized for the numerical integration of eq. (10) and (11), with the substitution of κ taken from eq. (16), in order to give the evolution of the

grain size d for continued plastic strain. This law is reported in Figure 3 in the solid line, while the dashed line represents the same integration but with $\kappa = \kappa_0$ as in the previous model we developed (Bacca *et al.* 2015)². On the abscissa is the shear equivalent plastic strain γ_p while on the ordinate is a logarithmic scale of the grain size ratio d / d_0 . Given the singularity of the function $d(\gamma_p)$ in its first derivative for $\gamma_p = \gamma_c$, which gives $d(\gamma_c) = -\infty$ (Bacca *et al.* 2015), we chose to integrate eq. (10) and (11) in an implicit form with respect to d so that we obtain the function $\gamma_p(d)$. This numerical integral has been calculated through a forward Euler method with a fixed step $\Delta d = -10^{-8} d_0$, initial value d_0 , up to the final value d_c . The latter value is asymptotically reached by the solid line of Figure 3 for very large γ_p as the rate of change of d , according to eq. (10) and (16), becomes 0 when $d = d_c$.

The evolution of the microstructure, in terms of grain refinement created by CDRX, has been observed experimentally by Shankar *et al.* (2005), and the grain size has been measured for three different amounts of plastic strain, as shown in Table 1. These results are indicated in Figure 3 with open circles and relative error bars ($\pm 50\%$) and compared with the curves discussed in the previous paragraph.

This figure shows that our current model gives excellent agreement with the experimental data, passing within the error bars for all the three experimental results. In addition, the figure shows how the current model, unlike the previous one (dashed line), captures the horizontal asymptote for the grain size at large plastic strains, at $d = d_c$.

Figure 3 also shows that a nanometric grain size such as d_c is the smallest obtainable by grain refinement caused by CDRX driven by plastic deformation. When such grain size is reached, GBS becomes a predominant deformation mechanism, and the system ceases to store energy in the microstructure. As a consequence, the driving force for the formation of new grain boundaries is negligible. At this point, the latent heat has saturated and no further grain refinement can occur.

In Figure 4 the evolution of the latent heat capacity is shown for the current model (solid line) and compared with that of our previous model (dashed line). These results are obtained from the ones shown with the solid line in Figure 3 through the use of eq. (16), for the proposed model in the solid line. A continuous decrease to zero is visible in the graph for the current model, which starts from the initial value of 0.12, while a constant value of 0.12 is assumed in our previous model.

Early experiments on the measurement of the latent heat were done by Taylor and coworkers. They believed the fraction of cold work being stored (as latent heat), as well as the fraction that is dissipated, was a constant material property. Later on it has been observed that these fractions are determined by the amount of plastic strain (Taylor and Quinney 1934); however, little influence has been noted in regards to strain rate (Hodowany *et al.* 2000). The temperature is also expected to play an important role in the energy storage, as high temperatures have the capability to release the latent heat by annealing. In the proposed model, the temperature has

² For this case analytical solution of eq. (10) and (11) can be obtained and is reported in Bacca *et al.* (2015).

been considered constant and close to its ambient room value. In support of this hypothesis most of the experiments considered, and performed at room temperature, have been observed to give a modest temperature rise (Farren and Taylor 1925, Rosenheim and Stott 1933, and Kanzaki 1951, Shankar *et al.* 2005), such that the mechanisms of energy storage and deformation are not affected by it.

In Figure 5 we show the evolution of the ratio of the dissipated heat Q to the amount of plastic work W_p done to the specimen for an increasing plastic strain. We call this ratio: the mean T&Q coefficient, and it is given by

$$\bar{\beta} = 1 - \frac{U_m}{W_p}, \text{ with } W_p = \int_0^{\gamma_p} \tau_y d\gamma_p, \quad (17)$$

The curve of $\bar{\beta}$ versus the shear equivalent plastic strain γ_p is shown by the solid line while the experimental results are shown by data points of various shapes. The theoretical results are obtained through substitution of eq. (11) into eq. (6) from the value of d shown in Figure 3, for U_m (see the description of Figure 7 for more detail), and by integration of eq. (8) and (9), for W_p . The experimental results are taken from Farren and Taylor (1925) (circles), Rosenheim and Stott (1933) (triangles), and Kanzaki (1951) (squares). All these authors used commercially pure aluminum specimens while the model has been calibrated to the machining experiments of Shankar *et al.* (2005), which uses Al6061-T6 specimens. Given the difficulties we encountered in retrieving experimental data on the specific alloy considered, we consider this comparison to be appropriate for a qualitative investigation as is well known that even minute amount of changes to the alloying composition result in relevant changes in the plastic behavior.

Figure 5 shows qualitative agreement between the theory and the experiments, and the experimental results are in qualitative agreement with each other. Farren and Taylor (1925) and Rosenheim and Stott (1933) performed mechanical tests in tension for a bar and a wire respectively, while Kanzaki (1951) performed compression tests on bars. These experiments were all carried out at room temperature but at different strain rates, we compare them by virtue of the negligible influence of the latter parameter on the phenomenon of energy storage (Hodowany *et al.* 2000).

In Figure 6 the T&Q coefficient is shown as a function of the shear equivalent plastic strain γ_p and is compared with experiments. The theoretical results are taken from Figure 4 by using eq. (5). The experimental results considered are taken from Mason, Rosakis and Ravichandran (1994) for Al 2024 specimens, and by Hodowany *et al.* (2000) for Al 2024-T3 specimens. Also in this case the materials are different from the one considered for the calibration of the model therefore the same consideration made for Figure 5 applies in this figure. Both sets of experimental results are obtained from high strain rate compression tests on a Kolsky bar. The comparison between the theory and the experiments should be limited to $0.85 \leq \beta \leq 1.00$ which is the range that is in agreement with the commonly accepted values from Taylor and coworkers (Farren and Taylor 1925, and Taylor and Quinney 1934). Within this range we observe a good matching for strains that are larger than 0.1 for Mason *et al.* (1994), and for strains larger than

0.4 for Hodowany *et al.* (2000). All three curves show a tendency towards a horizontal asymptote at $\beta = 1$, that corresponds to LHS.

In Figure 7 the evolution of the latent heat for continued plastic strain is shown for the current model (solid line) and compared with our previous model (dashed line). These results are obtained from the results shown in Figure 3. For each value of γ_p , its associated value of d is substituted into eq. (6) together with the result of eq. (11) to give the corresponding value for the latent heat U_m .

As evidenced by this figure, LHS leads to a continuous decrease in the slope of the curve until a steady state value (saturation) of the latent heat is obtained. Our previous model (Bacca *et al.* 2015), associated with the dashed line, did not capture this asymptotic behavior leaving the latent heat to increase indefinitely for continued plastic strain. The gap between the solid line and the dashed line represents the energy dissipated into heat by the increased GBS activity caused by grain refinement.

In Figure 8 we show the evolution of the deformation mechanism in terms of the ratio of the strain rate that is accommodated by GBS to the total strain rate. These results are obtained from the results shown in Figure 3. For each value of γ_p , its associated value of d is substituted into eq. (14).

In Figure 9, the ratio of the energy stored by the grain boundaries U_d (the second term on the right-hand side of eq. (6)) to the total latent heat U_m is shown as a function of plastic strain. These results are taken from the calculation made to obtain the results in Figure 7, by considering only the second term on the right-hand side of eq. (6) to obtain U_d . For an increasing plastic strain U_d increases as a fraction of the latent heat as more grain boundary surface is developed by grain refinement. An asymptotic value of 83.34 % is observed for this curve.

Stability of the nanostructure obtained by grain refinement, in metal alloys, is provided by second phase precipitates, which pins the grain boundaries inhibiting their annihilation created by grain growth. In these materials, the activation energy for grain growth can be much higher than the energy needed to activate recovery, which annihilates dislocations and releases their stored energy. As a consequence, grain refinement is especially desirable in metal alloys, as the latent heat redistribution shown in Figure 9 confers more stability to the increased hardness associated with the increase in latent heat obtained by cold working if compared to cold worked pure metals and metal alloys that have no grain refinement.

3.3 Finite element simulation of machining

The machining process involved in the experiments of Shankar *et al.* (2005) has been simulated with the finite element (FE) software Advant Edge (Third Wave Systems [<http://www.thirdwavesys.com/>]). In this simulation, the mechanical behavior of the material subject to plastic deformation is described by a user yield surface (UYS) and by a yield criterion. The YYS is a numerical algorithm that determines the value of the yield strength and other state variables for a given plastic strain. We encoded the proposed model as a YYS and choose the Von Mises yield criterion. In this case the yield strength in shear is obtained from eq. (8) for $\gamma_p \leq \gamma_c$, and

from eq. (9) for $\gamma_p > \gamma_c$ as shown in Figure 2. As state variables for the material, we chose to consider the microstructural parameter d and the energy storage parameters κ , β , U_m and U_d / U_m . The variable d can be evaluated numerically for a given plastic strain γ_p by integrating eq. (10) and (11), as reported in Section 3.2 and shown in Figure 3. With the purpose of reducing the computational time for the simulation, under the hypothesis of constant strain rate $\dot{\gamma}$ and temperature T , we introduce an explicit function $d(\gamma_p)$ that approximates the curve of Figure 3 with minimum discrepancy and provides the value of d for any given value of γ_p

$$d(\gamma_p) = \begin{cases} d_0 & \gamma_p \leq \gamma_c \\ d_0 + (d_c - d_0) \left\{ 1 - \exp \left[- \left(\frac{\gamma_p - \gamma_c}{\gamma_1} \right)^n \right] \right\} & \gamma_p > \gamma_c \end{cases} \quad (18)$$

where γ_1 and n are parameters that have to be calibrated in order to minimize the discrepancy between eq. (18) and the plot in Figure 3. For the case shown in Figure 3, associated with the machining experiment of Shankar *et al.* (2005), these parameters have values $\gamma_1 = 1.43 \cdot 10^{-5}$ and $n = 0.2$. It should be noted that eq. (18) is only a numerical approximation of the result of the model proposed in Section 2, therefore the reader should just take it as a suggestion for an explicit formulation of the function $d(\gamma_p)$ that has the purpose of save computational time. Moreover, if a different experiment is considered, *i.e.* a different set of strain rate $\dot{\gamma}$ and temperature T is adopted (holding the hypothesis of negligible temperature rise and constant strain rate), the parameters in Table 2-3 should be re-determined, eq. (10) and (11) should be integrated again with the new data and the values of the parameters γ_1 and n should be recalculated.

In Figure 10 we show the contour plot relative to the grain size d distribution for the machining simulation, by using eq. (18). The friction coefficient between the cutting tool and the chip is taken as 0.5, the cutting speed is chosen as the minimum allowed by the software, which is 20 mm/s (two times bigger than the cutting speed in Shankar *et al.* 2005, but still in the same order of magnitude), the rake angle is 20° , the feed a_0 (see Figure 1) is 0.15 mm, and the material of the specimen is the aluminum alloy Al6061-T6. Similarly, as observed by Bacca *et al.* (2015), relevant grain refinement takes place in the chip domain, including the primary deformation zone, as well as in a substrate that extends for 0.1 mm below the machined surface. In these regions, a minimum grain of $d_c = 100$ nm is shown in the blue contour. Outside these regions, the material has comparable properties with the same material in annealed conditions and is shown in the red contour. For the latter conditions, a grain size of $d_0 = 75$ μ m is considered, in agreement with Shankar *et al.* (2005).

Figure 11 shows the contour plot relative to the distribution of the latent heat capacity κ . The value of κ is obtained, for a given shear plastic strain γ_p , by substitution of d , taken from eq. (18), into eq. (16). A minimum value of 0 (which corresponds to LHS) is predicted within the regions of maximum grain refinement in the blue contour. The material in annealed conditions shows the maximum value of 0.12 in the red contour.

Figure 12 shows the contour plot relative to the distribution of the T&Q coefficient β . The value of β is obtained by substitution of κ , at the previous paragraph, into eq. (5). A maximum value of 1 (which corresponds to LHS) is predicted within the regions of maximum grain refinement in the red contour. The material in annealed conditions shows the minimum value of 0.88 in the cyan contour.

Figure 13 shows the contour plot relative to the distribution of the latent heat U_m . The value of U_m is obtained, for a given shear plastic strain γ_p , by substitution of d , taken from eq. (18), into eq. (11) and this, together with d , into eq. (6). A maximum value of $1.14 \cdot 10^7 \text{ J/m}^3$ is predicted within the regions of maximum grain refinement in the red contour. The material in annealed conditions shows the minimum value of $1.36 \cdot 10^6 \text{ J/m}^3$ in the blue contour. For the sake of comparison with experiments, the difference between the saturated latent heat and the latent heat in annealed conditions is considered as $\Delta U_m = 1 \cdot 10^7 \text{ J/m}^3$. Taking aluminum density as $\rho = 2.7 \cdot 10^6 \text{ g/m}^3$, we have $\Delta U_m = 0.88 \text{ cal/g}$, in agreement with the observations of Kanzaki (1951), and considering aluminum molar volume $V_m = 1 \cdot 10^{-5} \text{ m}^3/\text{mol}$, we have $\Delta U_m = 100 \text{ J/mol}$, in agreement with Saldana *et al.* (2012)³.

Figure 14 shows the distribution of the ratio of the latent heat stored by the grain boundaries U_d to the total latent heat U_m . The value of U_m is obtained as specified at the previous paragraph while, considering only the second term on the right-hand side of eq. (6), we have U_d . A maximum value of 83.34 % is predicted within the regions of maximum grain refinement in the red contour. This intuitively suggests that grain refinement is a process that builds a significant amount of grain boundary surface, from which, the grain boundary energy U_d . The material in annealed conditions shows the minimum value of 0.92 % in the blue contour, as in this condition, the latent heat of the material is stored primarily by the dislocation network.

4. Discussion

In the proposed model, the influence of the temperature, on grain refinement and on the evolution and mechanisms of energy storage, has not been investigated. The temperature is also expected to affect the critical grain size d_c , as relevant GBS has been observed for micrometric grain size in the form of high temperature creep (Langdon 1994). In this model, we adopted a constant average temperature that has a value sufficiently close to its room one T_r in order to allow us to neglect its influence on the studied phenomena. This hypothesis is supported by a negligible temperature rise observed in most of the experiments taken for comparison. Shankar *et al.* (2005) observed “negligible temperature rise” during their machining test, hypothesis confirmed by the study of Abolghasem *et al.* 2012, which measured a ΔT that is below 50°K , Farren and Taylor (1925) observed a temperature rise ΔT that is around 3°K ($0.01T_r$) and Rosenhein and Stott (1933) observed $\Delta T \approx 20^\circ\text{K}$ ($0.07 T_r$). A more relevant temperature rise, in the range of 100°K ($0.34 T_r$), is observed in the results of Mason *et al.* (1994) and Hodowany *et al.* (2000). In this regard, the comparison made in Figure 6 has to be considered qualitative. Thermal fluctuation in adiabatic conditions is also supposed to activate recrystallization for

³ Saldana *et al.* (2012) performed machining experiments on copper specimens, while the latent heat we calculated is related to an aluminum alloy. We expect to have a qualitative matching in this regard as the materials are different.

temperatures above $0.4 T_m$ (Meyers *et al.* 2003). Considering a final temperature of $350^\circ K$ (Abolghasem *et al.* 2012) and $0.4 T_m = 373^\circ K$ for aluminum, we consider this effect to be negligible for the purpose of this investigation.

The influence of strain rate has been considered indirectly in the proposed model. It is expected to affect the yield strength in shear at steady state τ_c , as well as the critical amount of shear equivalent plastic strain γ_c developed before τ_y reaches τ_c and CDRX begins. The value of τ_c has been obtained by the comparison with experimental measurement, on the Vicker hardness H_v , made by Shankar *et al.* (2005). In this way, the strain rate adopted in such experiment has been considered in the phenomena through calibration. The aforementioned authors did not directly measure the strain rate, however, an estimation has been done from the finite element simulation used to obtain Figures 9-13, and from empirical formulations, which gives a value of $\dot{\gamma} \approx 300 s^{-1}$. In Figures 5-6, the comparison between theoretical and experimental results is made with different strain rates. This comparison is supported by the little influence of the strain rate on the evolution of the T&Q coefficient observed by Hodowany *et al.* (2000). From this observation, we expect to obtain little influence from strain rate also on grain refinement, in virtue of the formulation obtained from the substitution of eq. (16) into eq. (5).

5. Conclusions

A description of the phenomenon of LHS has been provided in this paper. Its relationship with grain refinement due to CDRX has also been explained with the proposed thermodynamically consistent model. This model gives a phenomenological description of the microstructural evolution of polycrystalline materials, showing a final refined nanostructure obtainable with large plastic deformations. For metal alloys, this nanostructure is stable at room temperature and gives improved material properties that can be conserved at higher temperatures according to the design of the material. This stability is due to grain boundary pinning by second phase precipitates which, in this way, prevents the annealing phenomenon related to grain growth. Ultimately, this consideration underlines the importance of grain refinement in manufacture engineering and material science and stresses the importance of our study.

In the presented work, the temperature rise given by internal heat generation has been considered negligible. This hypothesis is supported by accordant observations found in the referred experimental work. This framework is extended from low to high strain rate compression and tension tests, and to low cutting speed machining. For different typologies of experiments, the temperature rise is expected to give relevant influence in the phenomena of study, thus it needs to be accounted.

If the temperature rise is neglected, a constant critical grain size d_c , for the inversion of the Hall-Petch effect, is considered for any amount of plastic strain. This grain size represents the asymptotic value for grain refinement, leading to the conclusion that a smaller grain size cannot be obtained with CDRX. As a consequence, no inverse Hall-Petch behavior is observed during grain refinement.

The evolution of the grain size, the latent heat and the T&Q coefficient, for continued plastic strain, is predicted by the proposed model and this prediction has been validated by experiments.

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Figure 1: Schematic representation of the machining experiment used for comparison of the proposed model. In this picture, the key parameters for machining are shown and their value for the experiment of Shankar *et al.* (2005) are reported in Table 1.

Figure 2: For experiments on machining, variation of the Vicker hardness H_v within the chip for various values of the shear equivalent plastic strain γ_p . The solid line indicates the model prediction while the experimental values are indicated with open circles and relative error bars. γ_c is the critical strain at which recrystallization begins. The material used in the experiments is the peak-aged Aluminum 6061, H_0 is the hardness prior to machining and H_c is the hardness of all the machined samples for which $\gamma_p > \gamma_c$. The Vickers indentation load is 50 g (Shankar *et al.*, 2005).

Figure 3: Evolution of the grain size d as a function of the shear equivalent plastic strain γ_p relative to the experiments in Figure 2. In the ordinate, we have the ratio d/d_0 in a logarithmic scale, where d_0 is the grain size at the annealed state. The solid line indicates the prediction made with the proposed model, with a microstructure dependent latent heat capacity $\kappa = \kappa(d)$, the dashed line indicates the prediction made with our previous model (Bacca *et al.* 2015) which assumes constant latent heat capacity $\kappa = \kappa_0$ (with κ_0 the value associated with zero plastic strain), and the open circles with error bars indicate the experimental results on machining (Shankar *et al.*, 2005).

Figure 4: Evolution of the latent heat capacity κ as a function of the shear equivalent plastic strain γ_p relative to the change in microstructure shown in Figures 3. The solid line indicates the prediction made with the proposed model, with a microstructure dependent latent heat capacity $\kappa = \kappa(d)$, while the dashed line indicates the prediction made with our previous model (Bacca *et al.* 2015) which assumes $\kappa = \kappa_0$.

Figure 5: Evolution of the mean Taylor & Quinney coefficient $\bar{\beta}$ as a function of the shear equivalent plastic strain γ_p relative to the change in microstructure shown in Figures 3. The solid line indicates the prediction made with the proposed model while the open polygons indicate the experimental values taken from Farren and Taylor (1925), Rosenhein and Stott (1933) and Kanzaki (1951).

Figure 6: Evolution of the Taylor & Quinney coefficient β as a function of the shear equivalent plastic strain γ_p relative to the change in microstructure shown in Figures 3. The solid line indicates the prediction made with the proposed model while the dashed lines indicate the experimental curves taken from Mason *et al.* (1994) and Hodowany *et al.* (2000).

Figure 7: Evolution of the latent heat U_m as a function of the shear equivalent plastic strain γ_p relative to the change in microstructure shown in Figures 3. The solid line indicates the prediction made with the proposed model, with a microstructure dependent latent heat capacity $\kappa = \kappa(d)$, while the dashed line indicates the prediction made with our previous model (Bacca *et al.* 2015) which assumes $\kappa = \kappa_0$.

Figure 8: Evolution of the ratio of the strain rate $\dot{\gamma}_{GBS}$ created by GBS to the total plastic strain rate $\dot{\gamma}_p$ as a function of the shear equivalent plastic strain γ_p relative to the change in microstructure shown in Figures 3.

Figure 9: Evolution of the ratio of the energy stored by the grain boundaries U_d to the total latent heat U_m as a function of the shear equivalent plastic strain γ_p relative to the change in microstructure shown in Figures 3.

Figure 10: Contour plot of the average grain size d for machining predicted with the finite element software Advant Edge (Third Wave Systems) [<http://www.thirdwavesys.com/>]. The friction coefficient between the cutting tool and the chip is 0.5, the cutting speed is 20 mm/s, the rake angle is 20° , the feed (a_0) is 0.15 mm, and the material of the specimen is Al6061-T6. The smallest value is 100 nm in the blue contour while the largest value is 75 μm in the red contour.

Figure 11: Contour plot of the latent heat capacity κ for machining. See Figure 9 for details on the simulation. The smallest value is 0 in the blue contour while the largest value is 0.12 in the red contour.

Figure 12: Contour plot of the Taylor and Quinney coefficient β for machining. See Figure 9 for details on the simulation. The largest value is 1 in the red contour while the smallest value is 0.88 in the cyan contour.

Figure 13: Contour plot of the Latent Heat U_m for machining. See Figure 9 for details on the simulation. The largest value is $1.14 \cdot 10^7$ in the red contour while the smallest value is $1.36 \cdot 10^6$ J/m³ in the blue contour.

Figure 14: Contour plot of the ratio of the latent heat stored by the grain boundaries U_d to the total Latent Heat U_m for machining. See Figure 9 for details on the simulation. The largest value is 83.34 % in the red contour while the smallest value is 0.92 % in the blue contour.