A reassessment of the dynamic thermomechanical conversion in metals

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Heat dissipation still remains an unsolved problem in dynamic plasticity, where nearly adiabatic conditions prevail during high-rate loading scenarios. It is well known that the mechanical energy that is not dissipated as heat during material straining remains stored in the lattice as microstructural defects, and thus a one-to-one relationship can be expected between the stored energy, the materials microstructure and its mechanical characteristics. This work demonstrates that this is not so straightforward. High-rate experiments on a Kolsky bar, combined with in situ thermal measurements, were performed on two well-studied materials: pure nickel and aluminum. A dislocation-based constitutive model was used to estimate the mechanical and thermomechanical material behavior. For both materials, the thermal response was observed to be strongly strain rate sensitive, while the mechanical flow, and microstructural characteristics (as characterized by transmission electron microscopy at similar strains), were not. This apparent discrepancy between mechanical and microstructural vs. thermal results is discussed, and the concept of thermomechanical conversion is reassessed.

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Dynamic (impact) failure of metallic solids may result in many, often unexpected accidental situations. Under such circumstances, one can observe specific dynamic deformation mechanisms. The short time scale of the dynamic loading is responsible for a temperature rise of the material due to the (near) adiabaticity of the problem [1]. One direct consequence of this phenomenon may be the potential thermal softening of the material and subsequent localization of the deformation, into the so-called adiabatic shear bands [2]. Despite this, not all of the mechanical energy spent into inelastic straining is converted into heat, and a further fraction - commonly known as the stored energy of cold work (SECW) [3] - remains stored in the material, particularly in the form of microstructural defects and arrangement thereof. One can thus calculate the fraction of inelastic work dissipated as heat - generally called the Taylor-Quinney factor [4, 5] (TQF or \( \beta_{int} \)) - just by solving the heat conduction equation, which after neglecting thermoelastic heating and assuming adiabatic conditions, reads [5]:

\[
\beta_{int} = \frac{\rho C \Delta T}{\int \sigma_{ij} d\varepsilon_{ij}^p} = \frac{Q}{W_p} \quad (1)
\]

where \( \rho \) is the material density, \( C \) is the heat capacity, \( \Delta T \) is the temperature rise, \( \sigma_{ij} \) and \( \varepsilon_{ij}^p \) are the components of the stress and plastic strain tensors, respectively; \( Q \) is the energy dissipated as heat, and \( W_p \) is the plastic or mechanical work.

Several earlier works [6–12] have identified the SECW - which can be calculated as the “1-\( \beta_{int} \)” fraction of the mechanical work - as a potential triggering mechanism for microstructural softening under dynamic conditions, which inevitably precedes material failure by shear localization. Less was reported in the literature about the rate sensitivity of the energy storage (or the heat dissipation), although a few works have partly addressed this issue [13–16]. Considering the significance of the thermomechanical coupling in dynamic material failure, one may wonder about the extent to which the stored energy of cold work can uniquely be predicted from a microstructural point of view.

It is well known that the amount of energy stored in a plastically deformed material is directly proportional to the evolving density of dislocations, inasmuch as these are the main contribution to the former [17]. The expression to estimate the volumetric stored energy in the material, where only short-range dislocation-dislocation interactions are considered, can be expressed as [18]:

\[
E_{stored} = \frac{1}{4\pi k} \ln \left( \frac{1}{2b\sqrt{\rho_{tot}}} \right) Gb^2 \rho_{tot} \quad (2)
\]

where \( k \) is 1 or (1-\( \nu \)), depending on the type of the dislocation (\( \nu \) being the Poissos ratio); \( b \) is the Burgers vector, \( G \) is the shear modulus, and \( \rho_{tot} \) is the total line dislocation density. Assuming a realistic value for the Burgers vector (2.5 Å), setting \( k=1 \), and varying the dislocation density between \( 10^{10} \) and \( 10^{15} \) m\(^{-2} \) (which may be characteristic of several processes of plastic deformation), the term “1/(4\( \pi k \)) ln (1/(2b\sqrt{\rho_{tot}}))” is shown to vary from 0.8 to 0.3. Consequently, Eq. 2 becomes [19]:

\[
E_{stored} = \alpha Gb^2 \rho_{tot} \quad (3)
\]

where \( \alpha \) is a constant of the order of 0.5, adjusted depending on the material. An estimation of the energy stored in a statically deformed metal, using two different dislocation-based hardening models, was done in [20], where a variant of Eq. 2 was used to compare the obtained analytical values with the measured ones from
differential scanning calorimetry (DSC). Though slightly underestimated, the predicted stored energy values were in good agreement with those measured by DSC. As to its dynamic counterpart, the stored energy of a dynamically deformed material was calculated by other authors through the measured increase of temperature during high speed deformation [21, 22]. There, the analytical estimation based on dislocation mechanics completely disagreed with the measured values of the energy storage. Specifically, in [22], the suitability of using Eq. 3 (or either Eq. 2) to calculate the SECW (and by consequence the TQF) under dynamic conditions was called into question. A different approach, based on the non-equilibrium thermodynamic theory of dislocation plasticity of Langer et al. [23–25], was applied in [26] on a finite element framework to compute locally the TQF for an adiabatic shear banding problem.

In this Letter we show by means of a counter-example that there is no unique and unequivocal relationship between the stress-strain characteristics, and hence the formation of shear bands, problem. A different approach, based on the non-equilibrium thermodynamic theory of dislocation plasticity of Langer et al. [23–25], was applied in [26] on a finite element framework to compute locally the TQF for an adiabatic shear banding problem.

A brief discussion about the mechanical model is presented here, with details provided in [22]. The material model itself considers dislocation cell structures and their evolution, in a two-phase approach: cell walls and cell interiors [27–30]. The former constitutes the hard phase, where dislocations are trapped and therefore their density is higher; the latter, in comparison with the cell walls, are nearly dislocation free. To accommodate gradients of plastic strain (lattice curvature) during deformation, the presence of geometrically necessary dislocations (GNDs) in the walls is considered too. Each population of dislocations have their own evolution expression, which combined by a rule of mixtures allows to calculate the total dislocation density:

\[
\rho_{\text{tot}} = f (\rho_w + \rho_{\text{GND}}) + (1 - f) \rho_c
\]

where \(\rho_w\) is the line dislocation density of the cell walls, \(\rho_c\) its counterpart of the cell interiors, \(\rho_{\text{GND}}\) is the line dislocation density of GNDs, while \(f\) is the volume fraction of the cell walls. A certain density of line defects in the microstructure will turn into a flow resistance at the macroscopic level, which under uniaxial loading and adopting the Taylor averaging model [31] reads:

\[
\sigma = M (\tau_0 + \tau)
\]

where \(M\) is the Taylor factor (equal to 3.06 for most FCC materials), \(\tau_0\) is a constant threshold lattice resistance \((\tau_0 = \sigma_0 / M)\), and \(\tau\) is the shear strength of the cell, which can be determined as:

\[
\tau = \alpha G b \left[ f \sqrt{\rho_w} + (1 - f) \sqrt{\rho_c} \right]
\]

Additional terms, such as temperature or strain rate sensitivity effects, may be included in Eq. 6 [22].

Therefore, the denominator of the TQF (Eq. 1) can be defined utilizing Eq. 5. To complete the expression analytically, and since no information about the temperature increment is provided, a thermodynamically-consistent heat generation is needed. In this work, we have used the formulation provided by Hakansson et al. [32], which is based on a crystal plasticity framework and was derived considering the latent-hardening into the free energy function. Using Taylor homogenization, i.e., considering all slip systems as equally active during deformation, and dividing the slip resistance into lattice friction \((\tau_0)\) and hardening (Eq. 6), the evolution of the heat dissipation with the microscopic strain can be computed as:

\[
dQ/d\gamma = |\tau_0 + \tau - \tau_b| \left(1 - \frac{\tau}{\tau_0 + \tau} + \frac{B}{\tau_0 + \tau} \frac{\tau}{\tau_0 + \tau} \right) + \chi \tau^2_b
\]

where \(\tau_b\) is the back-stress, \(\chi\) here is a factor controlling the amount of dissipated energy related to the back-stress; \(B\) is a material parameter connected with the saturation of the slip resistance, \(g\), the strain evolution of which follows:

\[
dg/d\gamma = (1 - B g) \left| \frac{\tau_0 + \tau - \tau_b}{\tau_0 + \tau} \right|
\]

The evolution of the back-stress, resulting from incompatibility in plastic deformation, i.e., internal stresses produced by the difference in the dislocation densities between the cell walls and the cell interiors, can be calculated as [33]:

\[
d\tau_b/d\gamma = k_r \frac{f}{1 - f} \alpha G b \left( \sqrt{\rho_w + \rho_{\text{GND}}} - \sqrt{\rho_c} \right) - k_r \tau_b
\]

where \(k_r\) is a constant controlling the back-stress recovery. Introducing the effect of internal stresses in the formulation provides information about the distribution of dislocations in the material, an approach that was already shown to give reasonable results on the prediction...
of the heat dissipation in dislocation dynamics calculations [34]. A summary of the parameters used to calculate Eq. 7, selected in accordance to experimental observations, can be found in Table I.

Concerning the experimental procedure, thermomechanical compression testing under high rate deformation was conducted on a split Hopkinson pressure bar (SHPB), made of φ19.4 mm C300 hardened maraging steel bars, combined with in situ thermal measurements by infrared (IR) detection. A 2-photocathode high-speed IR detector (HgCdTe & InSb), along with a 1:1 magnification optical system, was located facing the specimen. The data acquisition frequency of 2 MHz was fast enough to capture the transient events under SHPB testing. Radiation emitted from the specimen was collected by the IR detector, giving rise to a voltage signal, further reduced into the specimen’s surface temperature - see also [22]. Analogous configurations for high-speed thermal measurements were reported to succeed in previous works of these and other authors, e.g., [14, 16, 22, 35–41].

Cylinders for uniaxial SHPB compression loading were carefully machined from a φ12 mm Ni200 bar, in the as-received condition, and from an ingot of as-cast pure aluminum (Al 99.99%). Electron backscatter diffraction (EBSD) analyses were performed on the original materials following standard polishing procedures, with an Oxford NordlysNano detector in a Tescan MIRA-3 FEG scanning electron microscope. A proper selection of the magnification optical system, was located facing the specimen. The data acquisition frequency of 2 MHz was fast enough to capture the transient events under SHPB testing. Radiation emitted from the specimen was collected by the IR detector, giving rise to a voltage signal, further reduced into the specimen’s surface temperature - see also [22]. Analogous configurations for high-speed thermal measurements were reported to succeed in previous works of these and other authors, e.g., [14, 16, 22, 35–41].

Table I. Summary of the parameters used in the calculation of the heat dissipation (Eq. 7).

<table>
<thead>
<tr>
<th>Material</th>
<th>B</th>
<th>g_{initial}</th>
<th>χ (Pa^{-1})</th>
<th>k_r</th>
</tr>
</thead>
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<tr>
<td>Ni200</td>
<td>0.3</td>
<td>0.007</td>
<td>5e-10</td>
<td>40</td>
</tr>
<tr>
<td>Al99.99%</td>
<td>0.7</td>
<td>0.007</td>
<td>1e-9</td>
<td>40</td>
</tr>
</tbody>
</table>

Figure 1b shows the averaged mechanical response of Ni200 for the two strain rates under study. Though quite scarce in literature, comparable experimental results for analogous high-purity nickel can be found [44, 45]. A very similar work hardening behavior for both deformation velocities (strain rates) is evident here, indicating an apparent lack of strain rate sensitivity of the material in the high-rate regime, noting that strain rate effects in nickel may be more apparent when the initial grain size is scaled down to the nanocrystalline level [45, 46]. A comparable trend in terms of strain-rate sensitivity was observed for pure aluminum - see Fig. 1e, akin to the experimental results of other authors [40, 47]. Here we remark that the final microstructures of Ni200 (at a strain of 0.2) for both strain rates were similar, showing equiaxed dislocation cell structures with tangled boundaries, as known to form in deformed nickel [48]. No signs of recrystallization or other energy-consuming phenomenon were observed, as shown in Figs. 2a and 2c. The dislocation density was estimated from EBSD analysis [49] in the deformed specimens showing that, for both strain rates, the overall distribution is absolutely comparable (see Figs. 2b and 2d) - thus supporting both, the TEM results and the experimental strain rates for Ni200 (N prefix) an pure aluminum (A prefix).

Table II. Summary of the specimens’ dimensions and experimental strain rates for Ni200 (N prefix) an pure aluminum (A prefix).

<table>
<thead>
<tr>
<th>No. Spec.</th>
<th>L-φ(mm)</th>
<th>¯{ε} (s^{-1})</th>
<th>No. Spec.</th>
<th>L-φ(mm)</th>
<th>¯{ε} (s^{-1})</th>
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<tr>
<td>1 N20</td>
<td>4.97-5.01</td>
<td>3260</td>
<td>17 N39</td>
<td>4.93-5.00</td>
<td>4750</td>
</tr>
<tr>
<td>2 N22</td>
<td>4.97-5.00</td>
<td>3370</td>
<td>18 N42</td>
<td>4.87-4.97</td>
<td>4790</td>
</tr>
<tr>
<td>3 N24</td>
<td>5.06-4.97</td>
<td>3240</td>
<td>19 A32</td>
<td>8.01-8.00</td>
<td>3560</td>
</tr>
<tr>
<td>4 N25</td>
<td>5.00-5.00</td>
<td>3260</td>
<td>20 A36</td>
<td>8.04-8.00</td>
<td>3360</td>
</tr>
<tr>
<td>5 N67</td>
<td>5.98-5.97</td>
<td>3330</td>
<td>21 A37</td>
<td>8.01-7.98</td>
<td>3550</td>
</tr>
<tr>
<td>6 N77</td>
<td>4.94-5.01</td>
<td>3320</td>
<td>22 A40</td>
<td>8.02-8.00</td>
<td>3550</td>
</tr>
<tr>
<td>7 N78</td>
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<td>23 A41</td>
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<tr>
<td>8 N81</td>
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<td>3300</td>
<td>24 A42</td>
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<td>3500</td>
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<tr>
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<td>3650</td>
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<tr>
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<td>3270</td>
<td>26 A53</td>
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<td>5060</td>
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<td>4690</td>
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<td>4920</td>
</tr>
<tr>
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<td>4730</td>
<td>28 A56</td>
<td>7.84-7.98</td>
<td>4900</td>
</tr>
<tr>
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<td>4700</td>
<td>29 A58</td>
<td>8.04-8.07</td>
<td>4870</td>
</tr>
<tr>
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<td>4690</td>
<td>30 A59</td>
<td>8.00-8.00</td>
<td>5240</td>
</tr>
<tr>
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<td>5.02-5.00</td>
<td>4770</td>
<td>31 A60</td>
<td>8.04-7.98</td>
<td>5280</td>
</tr>
<tr>
<td>16 N34</td>
<td>5.03-5.00</td>
<td>4600</td>
<td></td>
<td></td>
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FIG. 1. Grain orientation maps, averaged stress vs. plastic strain (both experimental and predicted by Eq. 5), and averaged Taylor-Quinney factors ($\beta_{\text{int}}$) vs. plastic strain (both experimental and predicted by Eqs. 1 and 7), for a-c) Ni200 and d-f) Al99.99%. Experimental curves contain standard error bars.

analytical modeling. Specifically, the final average dislocation density for Ni200 samples deformed at a strain of 0.2 was determined to be $(3.46 \pm 2.32) \times 10^{14} \text{m}^{-2}$ at 3300 s$^{-1}$, and $(3.51 \pm 2.41) \times 10^{14} \text{m}^{-2}$ at 4700 s$^{-1}$. Following the similarities in the statistical characteristics of the dislocation density distributions, we further examined the distribution function by calculating their distance from each other utilizing Bhattacharyyas distance [50]. The latter was estimated as $8 \times 10^{-3}$, indicating that the two are practically identical irrespective of the strain rate; thus leading to the conclusion that the levels of stored energy are identical as well.

Figures 1c and 1f show the evolution of the inelastic heat fraction ($\beta_{\text{int}}$) during deformation. In this aspect, Ni200 and pure aluminum exhibit a definite thermomechanical sensitivity to the applied strain rate, in the sense that the amount of dissipated heat varies notably, e.g., for nickel, between 35 - 40 percent for the 3300 s$^{-1}$ case, and between 55 - 65 percent when the material is deformed at 4700 s$^{-1}$. Similar trends were obtained for aluminum. It can be noted that the thermal strain rate sensitivity is absolutely not captured by the dislocation-based model, whereas the mechanical response is properly estimated - see Figs. 1b and 1e.

These results lead to the following question: on what physical grounds, can a material that exhibits comparable dynamic mechanical properties irrespective of the strain rate and the microstructure, be creating such a contrasting amount of thermal power (heat rate) in each situation?

Other authors have reported without further emphasis a similar anomaly [15], where the dynamic thermomechanical response of an aluminum alloy was compared for several but close values of strain rate. The considerable thermal sensitivity presented there (TQFs varying between 0.4 and 0.95) is oppositely accompanied by milder changes in the mechanical flow characteristics; on the other hand, no microstructural data was collected there, thus a direct comparison with the work presented here is precluded. In the cases studied in this Letter, the rates of hardening for the two different strain rates in both materials were almost equal, respectively, as shown in Fig. 3. Yet, from the temperature rise per strain increment (in the same figure), one clearly sees that the heat generation rate surpasses the energy storing rate capacity of the material as the strain rate increases. Since no evident distinction between the final microstructure at the two strain rates was found (see Fig. 2), these observations can be understood as a counter-example of $\beta_{\text{int}}$ being solely a result of the final microstructure without accounting for its evolutions. Note here the claim made by Taylor and Quinney in 1934 [4], who suggested the in-
fluence of microstructural aspects on the material energy storage behavior prior to failure, a fact that has been lightly touched upon in literature since then.

While it would be highly desirable to monitor microstructural evolutions in real time at the dislocation scale, this eventuality is not achievable by nowadays experimental means. Yet, some conclusions can be drawn from the present observations, namely:

a) the ETMB dislocation model describes adequately the mechanical behavior of the two metals in question at both strain rates, while the thermal response - specially concerning the strain rate sensitivity - is not properly captured;

b) for the pure FCC metals studied here, there is no definite or unique relationship between the mechanical response (thus the final microstructure) and the stored energy of a dynamically deformed material;

c) the TQF is suggested to be rather influenced by the evolution of the microstructure and not by a final state of equilibrium, as commonly assumed, suggesting that dislocation kinetics and the dislocation structures evolution are of prime importance for understanding non-equilibrium deformation states and thermal dissipation, as suggested by Langer et al. [23].

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[43] The strain gages and the IR signals are recorded at different locations, and need to be carefully synchronized using the sound wave velocity in the bars (see Fig. 6a and explanations in [22]).


