On the dynamically stored energy of cold work in pure single crystal and polycrystalline copper

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Abstract

The thermo-mechanical response of single crystal and polycrystalline high purity copper is systematically compared at low and high strain rates. The mechanical response of each type of material is very different in terms of strain hardening, although both are distinctly strain rate sensitive. A simplified interpretation of the Taylor–Quinney coefficient, in which the strain dependence is not considered, shows a clear (almost linear) increase of this factor with the strain rate, while the two types show distinct trends. This factor increases with the strain rate but remains markedly lower than the classical value of 0.9. The stored energy of cold work is found to be relatively independent of the strain rate, with the polycrystal storing more energy than the single crystal. A microstructural study (transmission electron microscopy) of representative specimens of each type at low and high strain rates reveals a basically similar microstructure, despite dissimilar values of energy storage. It is proposed that a higher level of storage of the energy of cold work by polycrystalline copper is due to the presence of grain boundaries in this group.

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1. Introduction

It is a well-known fact that deformed crystalline solids tend to store part of the strain energy as what is called the stored energy of cold work (SECW). A comprehensive review of the subject can be found in Bever et al. [1]. The subject can be divided in two parts, namely static and dynamic loading. While a considerable body of work has been done on quasi-static loading configurations, less is known about the dynamics of energy storage in solids. A common denominator in dynamic loading experiments is that one needs to measure transient temperature changes which reflect the amount of dissipated energy, assuming that the situation is adiabatic in view of the typically short time and spatial scales. Temperature measurements are usually carried out by means of non-contact infrared pyrometry of specimens that are most often loaded by means of a Kolsky (split Hopkinson) apparatus [2]. The influence of these thermo-mechanical coupling effects has long been noted, considering for instance the evolution of so-called adiabatic shear bands in metals [3], during which the local temperature may increase dramatically. Based on the transient coupled heat equation [4], and assuming adiabatic conditions, the latter reduces after integration to:

\[
\beta_{\text{int}} \int_0^t \sigma_{ij} d\varepsilon_{ij}^p = \rho C_p \Delta T
\]

where \(\sigma\) is the stress tensor, \(\varepsilon^p\) the inelastic strain tensor, \(\rho\) is the density, \(C_p\) the heat capacity and \(\Delta T\) the temperature rise. The factor \(\beta_{\text{int}}\), in which the subscript \(\text{int}\) stands for integral [5], expresses the efficiency of conversion of mechanical into thermal energy, and is therefore smaller
than or equal to 1. At the same time the complementary process of energy storage (SECW), related to \(1 - \beta_{\text{int}}\), expresses the fact that the inelastic strain energy invested in a deforming solid is partly stored as SECW, which translates into microstructural rearrangements at the dislocation level. Dynamic energy storage has recently been singled out as the driving force for shear localization following dynamic recrystallization [6,7]. In this context one should mention the work of Benzerga et al. [8], who numerically modeled the storage of energy in copper single crystals, with an emphasis on the deformed microstructure, and specific consideration of the dislocation rearrangements (see also [9]). Experimental measurements of \(\beta_{\text{int}}\) require a synchronized measurement of the dynamic stress, strain, and temperature rise. Such measurements have been carried out for a few metals, alloys, and polymers. All these works yielded different values of \(\beta_{\text{int}}\) with the basic outcome that \(\beta_{\text{int}}\) is both strain and strain rate dependent [10–13], unless considered as a constant equal to 1, as in Kapoor and Nemat-Nasser [14]. These studies were inspired by the seminal contribution of Taylor and Quinney [15], as well as Farren and Taylor [16], who measured \(\beta_{\text{int}}\) in copper (unspecified grade) using high rate torsion and tension experiments. The temperature measurements were carried out using either small thermocouples or by calorimetric techniques (see also [17]). Since this historical measurement the Taylor-Quinney coefficient (\(\beta_{\text{int}}\)) is universally assumed to be \(\beta_{\text{int}} = 0.9\) for copper, a value which has since been generalized to all materials. The assumption of a constant \(\beta_{\text{int}} = 0.9\) (or 1) is convenient for numerical calculations as it provides an upper bound for the expected temperature rise during a high rate impact event. However, it can also sometimes be misleading when used automatically to justify very high local temperature rises that are not always physical.

Yet the experimental techniques have vastly improved since the days of Taylor, in the sense that high rate loading is almost a routine test using the Kolsky bar, while high speed infrared detectors provide a direct and accurate estimate of the temperature rise on the surface of a specimen [18]. Moreover, when moderate rates are considered, full field techniques, such as infrared cameras, can provide an accurate picture of the temperature distribution on the specimen.

In addition to polycrystalline materials, the investigation of single crystals is interesting, as they are representative of the elementary thermo-mechanical responses of polycrystals while supplying independent reference values as an input to numerical models of polycrystalline materials. Unfortunately, such studies are still scarce, with the exception of single crystal tantalum [17]. We note here that such studies on single crystals are of a necessarily limited nature due to the many combinations of slip systems that should be considered, thus amounting to a very large body of experiments in terms of initial specimen orientation.

The goal of the present work is therefore to re-examine the thermo-mechanical changes in pure copper, in both single and polycrystalline form, over a wide range of strain rates in order to produce a systematic comparison between the two, along with a detailed microstructural characterization.

The paper is organized as follows. We first present the materials and various experimental procedures, as well as the data reduction techniques. These techniques will be discussed here rather than in the discussion section. Next, results are shown for impact tests on single crystal and polycrystalline copper specimens, followed by similar results obtained in the rapid quasi-static regime. In the next section we report the results of a thorough complementary transmission electron microstructural characterization of the copper specimens, in order to shed additional light on the thermo-mechanical parameters measured in this work. The last section contains a discussion of the main results of this work, followed by concluding remarks.

2. Experimental

2.1. Material and specimens

The material of this study is basically high purity copper. Polycrystalline copper was purchased as OFHC copper rods and was tested in the as-received condition. Single crystalline high purity copper was purchased as (123) oriented cylinders. It can be shown that this orientation triggers single slip, at least at the onset of plastic deformation.

Both the single crystal and polycrystalline materials were supplied as cylindrical rods (6 mm diameter). Therefore, cylindrical specimens were carefully sectioned with a typical diameter of 6 mm, and a length of 4 or 6 mm to control the applied strain rate. All the specimens were tested in the as-received condition. A total of 23 OFHC specimens were successfully tested in the dynamic regime, while 5 were tested quasi-statically. A total of 13 single crystalline specimens were tested. 9 dynamically and 4 quasi-statically.

2.2. Mechanical and thermal testing

Mechanical testing was conducted in compression. Dynamic compression was carried out using 12.7 mm C300 maraging steel bars. The range of strain rates was \(\dot{\varepsilon} = 1000\text{–}8000\) s\(^{-1}\). The thermal measurements were carried out using a single element, liquid N\(_2\) cooled MCT detector. The set-up has been described elsewhere; for additional details see Rittel et al. [17]. It should be noted here that the thermal measurements were carried out over 100 × 100 \(\mu\)m areas. In addition to dynamic testing, quasi-static testing was carried out using an MTS system under displacement control. The system was used at relatively large cross-head velocities to avoid, as much as possible, heat loss to the surroundings. Here the typical strain rate was of the order of \(\dot{\varepsilon} \approx 1\) s\(^{-1}\). The thermal system consisted here of a FLIR Systems camera used in previous studies [17]. The recorded images were subsequently processed to extract the average surface temperature of the specimen. Note that
for both the quasi-static and dynamic experiments the thermal acquisition system was synchronized with the mechanical one such as to provide simultaneous stress, strain, and temperature recording.

2.3. Specimen thermal conditioning and calibration of the infrared detector

The infrared (IR) detector collects the radiation emitted by the specimen surface, which is measured as a voltage. The latter is then converted to a temperature (rise) via a thermal calibration procedure. This procedure consists of a comparison with the IR signal of a hot specimen into which a thermocouple has been inserted, so that a voltage–temperature plot is obtained. The measured thermal signal is known to be affected by the emissivity of the surface of the specimen. The latter varies continuously as the specimen deforms and the surface may become less reflective. It has also been argued that IR focusing is quite critical. It has also been argued that IR focusing is quite critical, although a recent reassessment of this issue shows that this is not the case [10,17,19,20]. We did not address the deformation-induced varying emissivity of the specimen, so that the error, if any, is deemed to be identical for all the dynamic tests. Moreover, it has been shown in several instances that for relatively low levels of strain, of the order of 0.2, the error is not significant. Another important point is that copper, like many other pure metals, has a high tendency to grow a thin surface layer of oxide when exposed to high temperatures. Consequently, if the calibration specimen is heated and then allowed to cool the signal is collected from a supposedly oxidized surface which is not present in the virgin specimen. To minimize errors that might be related to this state of affairs the specimens were deliberately preheated for 1 min with a hot air industrial blower, reaching temperatures of the order of 200 °C. This procedure was systematically applied to all the experimental and calibration specimens to ensure a uniform initial surface condition.

A very large number of calibrations were carried out, which typically consisted of five or more calibrations prior to testing, checking for repeatability before establishing the temperature–voltage conversion. This procedure was repeatedly applied to each new series of tests, among which random calibration checks were run to make sure that nothing had changed in the experimental set-up that could be attributed to, for example, loss of detector coolant fluid, falling detector battery tension or unwanted motion of the detector mirror system. As a result of the thorough calibration procedures the results presented here are deemed to be reliable and characteristic of the material response.

2.4. Determination of \( \beta_{int} \)

Based on Eq. (1) \( \beta_{int} \) is simply:

\[
\beta_{int} = \frac{\rho C b \Delta T}{W_p} \tag{2}
\]

where \( W_p \) is the plastic work density. However, as \( \beta_{int} \) is both a function of the strain and the strain rate it is usually reported as a function of the plastic strain for a given strain rate [10,11]. While such a representation is scientifically justified, it is nevertheless cumbersome when one would like to have a simple number that describes \( \beta_{int} \), such as 1 from Kapoor and Nemat-Nasser [14], or 0.9 from Taylor and Quinney [15]. Consequently, throughout this work \( \beta_{int} \) will be reported as the average slope of the temperature rise vs. plastic work density, as long as this slope is reasonably constant (linear relationship). It will thus be denoted by \( \beta_{av} \).

Another important issue which has been universally neglected so far relates to the exact determination of \( W_p \). While the latter is determined from the plastic strain (\( \varepsilon_p = \varepsilon_{total} - (\sigma/E) \)), it should be kept in mind that the initial elastic part of the dynamic stress–strain diagram is not accurately determined from the Kolsky bar experiment, as a result of a lack of dynamic specimen equilibrium. The plastic strain is therefore usually determined by truncating the obtained stress–strain curve. Throughout this work we overcame this issue by estimating and adding to the overall work density that initial part which is usually missing, as illustrated in Fig. 1. It will be noted here that this correction does not significantly affect the results since the \( \Delta T - W_p \) slope is not affected by this correction, the latter being carried out for the sake of completeness.

3. Results

3.1. Mechanical response of single and polycrystalline copper

3.1.1. Polycrystal

Fig. 2a shows typical true stress–strain curves obtained at various strain rates ranging from \( \dot{\varepsilon} = 0.1 \) to 7000 s\(^{-1}\). The material is observed to be strain rate sensitive, at least when comparing quasi-static with dynamic results. In the dynamic regime the material exhibits a more moderate level of strain rate sensitivity, in accord with previous studies on OFHC copper (see, for example, [21–23]). Note that in the quasi-static domain a noticeable apparent strain softening develops shortly after yielding. The reason for this behavior
is not clear, as some specimen buckling might be involved. Yet it should be noted that a similar response was observed by Rittel et al. [22], who used a different specimen geometry, a shear compression specimen (SCS).

3.1.2. Single crystal

Fig. 2b shows typical stress–strain curves for the single crystal specimens, in the range of strain rates of \( \dot{\varepsilon} = 0.1 \) to 5800 s\(^{-1}\). The material is observed to be strain rate sensitive, like polycrystalline copper, with pronounced strain hardening at all the investigated strain rates. For this material the apparent (proportional limit) yield strength of the single crystals is markedly inferior to that of the polycrystals.

3.2. Thermo-mechanical results

3.2.1. Dynamic tests

Fig. 3 shows a typical plot of the measured temperature rise as a function of the plastic work density (calculated with the correction shown in Fig. 1). The relationship is reasonably linear, and \( \beta_{\text{int}} \) can be determined from the slope of the graph, as mentioned before. In that case \( \beta_{\text{int}} \) is to be understood as an average representative value (\( \beta_{\text{av}} \)), much in the sense of the values reported by Taylor and Quinney [15].

Fig. 4a summarizes the results for the measured \( \beta_{\text{av}} \) in the high strain rate regime for the single crystal and polycrystalline materials. The first observation is that \( \beta_{\text{av}} \) is nearly linearly dependent on the strain rate in the range of strain rates investigated here. The polycrystalline and single crystalline copper exhibit the same linear trend, but the polycrystal exhibits smaller \( \beta_{\text{av}} \) values.

Another observation, perhaps the most striking, is that the polycrystalline copper shows values of \( 0.5 \leq \beta_{\text{av}} \leq 0.7 \), which is far below the commonly accepted constant value of 0.9. Such a value may perhaps be reached (by extrapolation) only for much higher strain rates.

3.2.2. Quasi-static tests

These tests consisted of compressing cylinders while using a full field IR camera to monitor the surface temperature, then calculating the average and processing it to \( \beta_{\text{av}} \) as described previously. Here we will make the assumption, to be discussed in the sequel, that these tests can be considered as being carried out under adiabatic conditions. Fig. 4b shows a summary of \( \beta_{\text{av}} \) for both the single crystal and polycrystalline Cu. This figure again shows what seems to be a linear relationship between \( \beta_{\text{av}} \) and the strain rate, as in the dynamic regime. However, here the tendency is inverted in the sense that the \( \beta_{\text{av}} \) values of the single crystals are lower than those of the polycrystals. The exact reasons for this observation are not clear at this stage.

3.2.3. Comparison of the thermo-mechanics of single crystal and polycrystalline copper

It is interesting to compare the results obtained so far for the two kinds of copper, so as to outline the commonalities and differences between the two. Fig. 5 shows the evolution of temperature as a function of the plastic work density. Note that the slope of the curve corresponds to the average value of \( \beta_{\text{int}} \).
density in the dynamic regime. The relationship is reasonably linear for the two materials. The slopes are globally different, corresponding to different $\beta_{av}$ values. Note that for both cases the curves could all be lumped into one curve by shifting their intercept with the $x$-axis. This intercept corresponds to the uncertainty in determination of the initial plastic work density due to uncertainties in the measured elastic part of the stress–strain curve, as discussed earlier. Fig. 6 shows similar results for the quasi-static experiments. Here, in contrast, two groups of slopes can be identified according to the range of strain rates. The steeper slopes (higher $\beta_{av}$) correspond to the larger strain rates, which are probably closer to the adiabatic regime.

One can also note that the relationship between the temperature rise and the plastic work density is reasonably linear for the polycrystal, whereas the linearity is more limited for the single crystals. This may also be related to some lateral buckling (shear) that developed during the later stages of compression of the single crystals. Here again, the curves could be shifted horizontally such as to form two clear clumps for each range of strain rates. Altogether, these figures reveal a clear similarity in the relationship between the temperature rise and the plastic work rate, according to the range of strain rates considered, irrespective of the crystalline nature of the copper specimens.

One can now summarize the results for $\beta_{av}$ over the whole range of investigated strain rates by comparing Fig. 4a and b. For the single crystalline material a discontinuity in the linear relationship between $\beta_{av}$ and strain rate is apparent. This discontinuity is less apparent for polycrystalline copper due to the large spread in measured $\beta_{av}$ values in the quasi-static regime. The inherent nature of the quasi-static tests, carried out at relatively high crosshead velocities, and the variability in the results obtained for the polycrystal do not allow firm conclusions to be drawn. However, in view of all the other similarities between the polycrystalline and single crystalline thermal response it seems reasonable to assume that there is a discontinuity of slope in the $\beta_{av}$ strain rate in the quasi-static regime, the latter being more pronounced for the single crystal specimens. It is nevertheless clear that additional experimental work is required to ascertain the existence of such a discontinuity.
3.2.3.1. Strain rate dependence of the Taylor–Quinney factor and its value. To summarize this section, our results show that $\beta_{av}$ is nearly linearly dependent on the strain rate for both the single crystal and polycrystalline copper, at least in the high strain rate regime. On average polycrystalline Cu exhibits smaller $\beta_{av}$ values. This also indicates that at comparable strain rates polycrystalline Cu will store more energy of cold work than its single crystalline counterpart. Finally, the expected $\beta_{av}$ value of 0.9 was not found in this study.

3.3. Microstructural characterization

The microstructure of selected single crystal and polycrystalline specimens was characterized using optical microscopy and transmission electron microscopy (TEM). This step is a necessary link between the thermodynamic concept of stored energy and the material microstructure in fine detail.

3.3.1. Single crystal quasi-static loading ($\dot{\varepsilon} \approx 0.1 \text{ s}^{-1}$)

The microstructure of single crystalline copper statically compressed to 50% strain consists of dislocation cells and dislocation tangles. The cell size is approximately $\ldots$
0.5–1 μm. The cell interior is not free of dislocations (Fig. 8a). This microstructure is consistent with the beginning of stage III (parabolic) of work hardening, where more than four slip systems are active. The detailed structure of cell walls is shown in Fig. 8b. Within the boundaries the dislocations form tangles or wavy arrays, which is also consistent with the beginning of stage III.

3.3.2. Single crystal dynamic loading ($\dot{\varepsilon} \approx 6500 \text{ s}^{-1}$)

Dynamically deformed single crystals (50% strain) exhibit a microstructure that is quite similar to that of the quasi-statically deformed crystals. The microstructure consists of dislocation cells, as can be seen in Fig. 8c. The dislocation cell size is approximately 0.5–1 μm. As before, the dislocation cell interior is not free of dislocations, which corresponds to the beginning of stage III.

The internal structure of dislocations within the boundaries consists of tangles and wavy arrays (Fig. 8d).

3.3.3. Polycrystals quasi-static loading ($\dot{\varepsilon} \approx 0.1$ and 1.2 s$^{-1}$)

Three polycrystalline quasi-static samples were examined, which were deformed to 25% strain. All were observed to exhibit a similar microstructure. The initial grain size is relatively small (≤10 μm). It was also observed that the microstructure contains annealing (not to be confused with deformation) twins, with a typical width of a few microns.

The microstructure of statically deformed copper polycrystals consists of dislocation cells and a few second generation microbands, consistent with previous observations of compressed polycrystalline copper [24]. The cell size is 0.5–1 μm, and the microband width is approximately 0.3 μm. The cellular structure is shown in Fig. 9a. This structure corresponds to the beginning of work hardening stage III, where more than four slip systems are active. The detailed internal structure of dislocation cell boundaries again consists of arrays of wavy dislocations, as shown in Fig. 9b.

3.3.4. Polycrystals dynamic loading ($\dot{\varepsilon} \approx 2000 \text{ s}^{-1}$)

The microstructure of dynamically compressed polycrystalline copper (25% strain) is similar to that of the statically deformed material. The microstructure consists of dislocation cells, dislocation tangles and a few second generation microbands. Fig. 9c shows dislocation cells, and dislocation tangles can be seen in Fig. 9d. This microstructure is again consistent with observations of the beginning of work hardening stage III. In the same manner, the detailed internal structure of dislocation cell boundaries consists of arrays of wavy dislocations, as shown in Fig. 9d.

3.4. Microstructural comparison

3.4.1. Single crystal static vs. dynamic deformation

The microstructure of statically and dynamically deformed single crystalline copper is essentially similar. It basically consists of dislocation cells and dislocation tangles typically observed in the beginning of stage III of work hardening.

3.4.2. Polycrystal static vs. dynamic deformation

The same degree of similarity is also observed for polycrystalline copper. In both cases the microstructure consists of dislocation cells, dislocation tangles and second generation microbands.
generation microbands, which are usually observed in statically deformed polycrystalline copper above 0.1 strain.

3.4.3. Single crystal vs. polycrystal static and dynamic deformation

The detailed microstructural study indicates that the resulting microstructures of single crystal and polycrystalline specimens is virtually identical (except for the presence of a few microbands), irrespective of the rate of deformation.

Considering the large differences in the measured values of their respective $\beta$ factors (Fig. 4), this overall resemblance may seem surprising, and this point will be addressed in the Discussion section, where it will be shown that the microstructural similarity is expectable and natural.

4. Discussion and summary

This work represents an attempt to investigate and characterize the thermo-mechanical responses of high purity copper in the single and polycrystalline forms. Similar studies are scarce, except perhaps for the case of tantalum [17], although this study did not include a thermal characterization at low strain rates. One should also note the detailed parallel microstructural characterization, which is central in understanding the results presented in this work.

Before discussing and summarizing the main results of this work it should be remembered that the results reported for the single crystal copper are necessarily of a limited nature since only one orientation was considered. Therefore, these results should be considered as a partial description of the global single crystal response of this material. The discussion will not address the purely mechanical results, as such results can easily be found in the literature, and the current ones (for OFHC) are not an exception.

The main issue here is determination of the Taylor–Quinney coefficient from a more engineering oriented perspective, with the underlying question of whether it can be represented by a single value, e.g. 0.9. In this work we have adopted a different approach to $\beta_{av}$ where the strain dependence of this factor was deliberately set aside for simplicity reasons and an average value was reported for each strain rate, which was determined according to its definition, namely the slope of the temperature rise–plastic work density relationship. By doing so it is believed that the result is both more practical from an engineering point of view as a constant is measured and also more comparable with the seminal results of Taylor and Quinney [15]. However, the results obtained in this work show that the quasi-universal assumption $\beta_{int} = 0.9$ falls relatively far from what was measured here for polycrystalline copper. Finding a straightforward explanation for this discrepancy is difficult, except for the fact that Taylor and Quinney’s [15] method of measurement was indirect and perhaps less accurate than the use of modern IR detectors, which does not detract from the pioneering character of their work.

It was observed that the single crystal and polycrystalline copper specimens are characterized by different $\beta_{av}$. In spite of this difference, Fig. 4 reveals a very similar dependence of $\beta_{av}$ on the strain rate, noting that the relationship is nearly linear in the dynamic regime. The lack of similar studies on other materials precludes a generalization of this observation to other metallic materials, so that

Fig. 9. TEM micrographs of polycrystals deformed to 25%. (a) Quasi-static, low magnification image of dislocation cells (arrowed) and tangles. (b) Quasi-static, high magnification of the detailed wavy arrangement of dislocations (arrowed) within the cells boundaries. (c) Dynamic, low magnification view of dislocation cells (arrowed). (d) Dynamic, high magnification of the detailed structure consisting of wavy dislocations (arrowed).
the observed linear relationship is strictly valid for copper, but should certainly be further verified for other materials. Yet it is interesting to note that for tantalum [17] the opposite trend was observed, namely the polycrystal exhibited higher $\beta_{av}$ values than the two orientations of single crystals tested. For Ta it has been mentioned that twinning may be active at high strain rates [25], which is not the case for the Cu samples tested here. Our previous study on Ta did not involve microstructural characterization. As mentioned by Bever et al. [1] and observed by Padilla et al. [26], twinning is a deformation mechanism that does not store significant amounts of SECW, so that (dissipative) twinning is associated with high $\beta$ values. Therefore, one could tentatively rationalize the different behaviors of Ta and Cu by invoking twinning in polycrystalline Ta at high strain rates, which in any case calls for additional thermo-mechanical studies with in-depth microstructural characterization.

As to Cu, one should note that in the quasi-static regime there seems to be a break in the linear $\beta_{av} - \dot{\varepsilon}$ relationship, at least for the single crystals and also perhaps for the polycrystalline copper, at low strain rates, as is evident on comparing Fig. 4a and b. Note that the $\beta_{av}$ values measured for the single crystal show relatively good agreement with those calculated from the discrete dislocation plasticity by Benzeraga et al. [8]. The natural question which arises here relates to whether the rapid quasi-static tests can be considered to be adiabatic. To address this issue one may refer to the analysis by Rabin and Rittel [27] of the temperature gradient in cylindrical specimens subjected to uniform bulk heat generation. The results, reported in non-dimensional form (Biot vs. Fourier numbers), analyze the temperature gradient that may develop between the core and the surface of the specimen where heat convection effects are active. Based on this work, the Biot number can be estimated as $Bi = 10^{-4}$. Given $s = 1.12 \times 10^{-4}$ m$^2$ s$^{-1}$ (thermal conductivity), $R = 3$ mm (specimen radius), and a time lapse of 0.5 s $\leq \tau \leq 5$ s one obtains a corresponding Fourier number in the range $6.3 \leq Fo \leq 63$. According to Rabin and Rittel [27] for such a low Biot number the relative temperature difference between the core and the surface of the specimen is less than 5%. In such a case heat convection has almost no effect on the temperature distribution, which in turn suggests that the test can be considered to be adiabatic (negligible $kV^2T$).

Considering now the SECW, the microstructural characterization was carried out to shed additional light on the relationship between deformation micro-mechanisms, strain rate and/or strain, and energy storage [1,26]. Here the most surprising result is that in spite of the significant differences in their $\beta$ factors all the investigated specimens exhibit an apparently highly similar microstructure, whether single crystal or polycrystalline, and irrespective of the strain rate. This similarity includes comparable cell sizes irrespective of the strain rate for the two materials. This parameter evolves with strain, strain rate, and temperature, reaching a saturation state, which seems to be the case in the present work. Note that the cell size appears as a parameter in constitutive material models at high strain rate [28].

At this stage one must note that the comparison deals with polycrystals which were strained to only 25%, compared with 50% for the single crystals. The strain which is required to produce a similar microstructure is higher for single crystals, for which the operation of multiple slip systems occurs at higher strain compared with polycrystals, where several slip systems are readily active with the onset of plasticity [24,29].

However, the meaning of this observation can be further refined by distinguishing the bulk material, e.g. the dislocation cells in the two materials, and the grain boundaries only present in the polycrystal. The reported microstructural resemblance obviously refers only to the bulk material, as grain boundaries are absent in the single crystals. Based on the relative insensitivity of the stored energy on the strain rate, the identical bulk microstructures in the single crystal and polycrystalline copper specimens (at comparable levels of strain, or rather cell size) should be contrasted with the larger amounts of stored energy in the polycrystal. Looking at Fig. 7, a first estimate shows that the polycrystal stores roughly twice as much energy of cold work than does the single crystal. To explain this discrepancy one can suggest that the additional (excess) stored energy in the polycrystal is in fact essentially stored in the grain boundaries, as the latter are well-known to be sources of sinks for dislocations, as a result of plastic incompatibility between grains. The partition of stored energy into two terms, one being bulk storage (single crystal) and the second being identified as the grain boundary contribution, has not been quantified in previous work to the best of our knowledge.

One can thus summarize this work as a joint thermo-mechanical–microstructural study of the thermo-mechanics of copper, which first shows a clear dependence of the Taylor–Quinney factor on the strain rate (almost linear), while the strain dependence itself has not been addressed. The first obvious result is that $\beta_{int}$ is not equal to a constant value of 0.9 as previously accepted. It is also shown that for two distinct sets of microstructure (single crystal and polycrystalline) the SECW depends almost linearly on the plastic strain for each class of materials, while for each class all the strain rates can be lumped into a single “master curve”. For a given level of plastic strain, irrespective of the strain rate, the polycrystalline Cu stores more energy that the single crystal. Parallel microstructural (TEM) characterizations show a remarkable resemblance of all the bulk microstructures, again without a dependence on the strain rate. Within a given group the resemblance is expected to be due to a lack of dependence on the strain rate. Between the two groups the strong microstructural resemblance coupled to the different capabilities in terms of energy storage can be ascribed to the presence of grain boundaries in the polycrystalline samples.
5. Conclusions

A systematic comparative study was carried out on the thermo-mechanical responses and properties of single crystal and polycrystalline high purity copper. The following conclusions can be drawn from this work.

1. The mechanical responses of each class are very different in terms of strain hardening, although both are distinctly strain rate sensitive.
2. A simplified interpretation of the Taylor–Quinney coefficient ($b_{int}$) in which the strain dependence is not considered shows a clear (almost linear) increase of this factor with the strain rate in the dynamic regime, while the two groups show distinct trends.
3. The SECW depends almost linearly on the plastic strain for all the investigated strain rates. Yet all the curves can be collapsed into a single curve, indicating a relative independence on the strain rate. Again, each group shows a distinct behavior.
4. A TEM microstructural study of representative specimens of each group at low and high strain rates shows a basically similar microstructure. This can firstly be explained by the independence of the level of stored energy on the strain rate.
5. It is proposed that a higher level of SECW by the polycrystalline copper is due to the presence of grain boundaries in this group.
6. It is therefore suggested similar studies on other materials are carried out to pinpoint the individual contributions of the bulk material and the grain boundaries to the overall process of energy storage.

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