ON THE DYNAMICALLY STORED ENERGY OF COLD WORK IN PURE SINGLE AND POLYCRYSTALLINE COPPER

D. Rittel[1*], A.A. Kidane[2], M. Alkhader[2], A. Venkert[3], P. Landau[3] and G. Ravichandran[2]

(1) Faculty of Mechanical Engineering, Technion, Haifa, Israel
(2) GALCIT, California Institute of Technology, Pasadena CA, USA
(3) Department of Physics, NRCN, Beersheva, Israel

ABSTRACT

The thermomechanical response of single 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 on the strain-rate, with the polycrystal storing more energy than the single crystal.
Microstructural study (TEM) 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 higher level of storage of energy of cold work by the polycrystalline copper is due to the presence of grain-boundaries in this group.

KEYWORDS: Copper, Taylor-Quinney coefficient, stored energy, strain-rate, microstructure.

(*) Corresponding author: merittel@technion.ac.il

1. INTRODUCTION

It is a long known fact that deformed crystalline solids tend to store part of the strain energy into 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 to 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 those thermomechanical coupling effects has long been noticed, considering for instance the evolution of the 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:

$$\beta_{\text{int}} \int_0^{\alpha} \sigma_{ij} d\varepsilon_{ij}^{p} = \rho C_p \Delta T \qquad (1)$$

Where σ is the stress tensor, ε_p the inelastic strain tensor, ρ is the density, Cp the heat capacity and ΔT the temperature rise. The factor β_{int} , where the subscript *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- β_{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. The dynamic energy storage has been recently 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 modeled numerically the storage of energy into copper single crystals, with emphasis on the deformed microstructure, and specific consideration of the dislocations' rearrangements (see also Longere and Dragon [9]). Experimental measurements of β_{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 β_{int}, with the basic outcome that β_{int} is both strain and strain-rate dependent [10-13], unless considered as a constant equal to 1, like 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 β_{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 Rittel et al. [17]). Since this historical measurement, the Taylor-Quinney coefficient (β_{int}) is universally assumed to be β_{int} = 0.9 for copper, a value which has since then been generalized to all materials. The assumption of a constant β_{int} =0.9 (or 1) is quite convenient for numerical calculations as it provides an upper bound for the expected temperature rise during a high rate impact event. But 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 evolved since G.I. Taylor's days, 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 elevation 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 material, the investigation of single crystals is very interesting, as representative of the elementary thermomechanical response of the polycrystal, 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 thermomechanical conversion 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 and polycrystalline copper specimens, followed by similar results obtained in the rapid quasi-static regime. In the next section, we report the results of the thorough complementary transmission electron microstructural characterization of the copper specimens, in order to shed additional light on the thermomechanical parameters measured in this work.

The last section contains a discussion of the main results of this work, followed by concluding remarks.

II EXPERIMENTAL

II.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 single 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 mm 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, out of which 9 dynamically and 4 quasi-statically.

II.2 Mechanical and thermal testing

Mechanical testing was conducted in compression. Dynamic compression was carried out using 12.7mm C300 maraging steel bars. The range of strain rates was $\dot{\varepsilon} = 1000 - 8000\, s^{-1}$. The thermal measurements were carried out using a single element, liquid N2 cooled MCT detector. The setup was described in previous publications, and the interested reader can refer to Rittel et al. [17] for additional details. It will just be precised that the thermal measurements were carried out over 100μmx100μm 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 crosshead velocities to avoid, as much as possible, heat losses 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 again 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 the dynamic experiments, the thermal acquisition system was synchronized with the mechanical one such as to provide a simultaneous stress-strain-temperature recording.

II.3 Specimen's thermal conditioning and calibration of the infrared detector

The infrared detector collects the radiation emitted by the specimen's 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 comparing 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, although a recent re-assessment 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 a virgin specimen. To minimize errors that might be related to this state of affairs, the specimens were deliberately preheated for 1 minute with a hot-air industrial blower, reaching temperatures of the order of 200C. 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 5 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 setup, that could be attributed e.g. to loss of detector coolant fluid, dropping 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's response.

II.4 Determination of β_{int}

Based on eqn. (1), β_{int} is simply:

$$\beta_{\text{int}} = \frac{\rho C_p \Delta T}{W_p} \qquad (2)$$

Where W_{p} is the plastic work density. However, as β_{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 β_{int}, such as 1 from Kapoor and Nemat-Nasser [14], or 0.9 from Taylor and Quinney [15]. Consequently, throughout this work, β_{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 $\beta_{ave.}$

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 ($\varepsilon_p = \varepsilon_{total} - \frac{\sigma}{E}$), 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 Figure (1). It will be noted here that this correction does not affect significantly the results since the ΔT- W_{p} slope is not affected by this correction, the latter being carried out for the sake of completeness.

III RESULTS

III.1 Mechanical response of single and polycrystalline copper

a. Polycrystal

Figure 2(a) shows typical true stress-strain curves obtained at various strain rates ranging from $\dot{\varepsilon} = 0.1 - 7000\, s^{-1}$. The material is observed to be strain-rate sensitive, at least when comparing quasi-static to 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 e.g. [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 incriminated. Yet, it should be noted that a similar response was observed by Rittel et al. [22] who used a different specimen geometry, the shear compression specimen (SCS).

b. Single crystal

Figure 2(b) shows typical stress-strain curves for the single crystal specimens, in the range of strain rates of $\dot{\varepsilon} = 0.1 - 5800\, s^{-1}$. The material is observed to be strain-rate sensitive like the polycrystalline copper, with a 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.

III.2 Thermomechanical results

III.2.1 *Dynamic tests*

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

Figure 4(a) summarizes the results of the measured β_{ave} in the high strain-rate regime for the single and polycrystalline material. The first observation is that β_{ave} is rather linearly dependent on the strain-rate, in the range of strain-rates of this investigation. The polycrystal and the single crystalline copper exhibit the same linear trend, but the polycrystal exhibits smaller β_{ave} values.

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

III.2.2 *Quasi-static tests*

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

III.2.3 *Comparison of the thermomechanics of the single and polycrystalline copper*

It is interesting to compare the results obtained so far for the two kinds of copper, such as to outline the commonalities and differences between the two. Figure 5 shows the evolution of the temperature as a function of the plastic work density in the dynamic regime. The relationship is reasonably linear for the two materials. The slopes are globally different, corresponding to different β_{ave} 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 the determination of the initial plastic work density due to uncertainties in the measured elastic part of the stress-strain curve, as discussed earlier. Figure 6 shows similar results for the quasi-static experiments. Here, by contrast, two groups of slopes can be identified according to the range of strain-rates. The steeper slopes (higher β_{ave}) 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 at the later stages of the compression of the single crystals. Here again,

curves could be shifted horizontally such as to form 2 clear lumps at 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 β_{ave} over the whole range of investigated strain-rates by comparing Figures 4(a) and 4(b). For the single crystalline material, a discontinuity in the linear relationship between β_{ave} and the strain rate is apparent. This discontinuity is less apparent for the polycrystalline copper due to the large spread in measured β_{ave} 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 for firm conclusions to be established. However, in view of all the other similarities between the poly and single-crystalline thermal response, it seems reasonable to assume that there is a discontinuity of slope in the β_{ave}-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.

Strain-rate dependence of the Taylor-Quinney factor and its value

To summarize this section, our results show that β_{ave} is rather linearly dependent on the strain-rate for both the single and polycrystalline copper, at least in the high strain-rate regime. On the average, polycrystalline Cu exhibits smaller β_{ave} values. This also indicates that, at a comparable strain-rate, the polycrystalline Cu will store more energy of cold work than its single-crystalline counterpart. Finally, the expected β_{ave}=0.9 value is not measured in this study.

On the stored energy of cold work: strain-rate and strain dependence

Figure 7 shows the stored energy of cold work as a function of the plastic strain, at various strain-rates, for the 2 material conditions. The SECW does not show a strong dependence upon the strain-rate for each material. Consequently, for each group of materials, these curves can all be collapsed into a single curve (dashed trendlines), as a first approximation. The stored energy of cold work is observed to increase with the plastic strain, while being consistently superior for the polycrystalline copper, as

expected. In other words, irrespective of the strain-rate, at a given plastic strain the polycrystalline copper stores significantly more energy of cold work than the single crystal.

III.3 Microstructural characterization

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

III.3.1 *Single crystal – quasi-static loading* ($\dot{\varepsilon} \approx 0.1 s^{-1}$) – Figure (8a, b)

The microstructure of single crystalline copper, statically compressed to 50% strain, consists of dislocation cells and dislocation tangles. The cell size is approximately 0.5-1μm. The cell interior is not free of dislocations (Figure 8(a)). This microstructure is consistent with the beginning of stage III (parabolic) of work hardening, where more than 4 slip systems are active. The detailed structure of cell walls is shown in Figure 8(b). Within the boundaries, the dislocations form tangles or wavy arrays, which is also consistent with the beginning of stage III.

III.3.2 *Single crystal – dynamic loading* ($\dot{\varepsilon} \approx 6500 s^{-1}$) - Figure (8c, d)

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 Figure 8(c). The dislocation cell size is approximately 0.5-1μm. Like 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 (Figure 8(d)).

III.3.3 *Polycrystals – quasi-static loading* ($\dot{\varepsilon} \approx 0.1 \, and \, 1.2 s^{-1}$) – Figure (9a, b)

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 (≤10μm). It was also observed that the microstructure contains

annealing (not to be confused with deformation) twins, with a typical width of 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 0.5-1μm, and the microband width is approximately 0.3μm. The cellular structure is shown in Figure 9(a). This structure corresponds to the beginning of the third stage of work hardening, where more than 4 slip systems are active. The detailed internal structure of dislocation cell boundaries consists again of arrays of wavy dislocations, as shown in Figure 9(b).

III.3.4 *Polycrystals – dynamic loading* ($\dot{\varepsilon} \approx 2000\, s^{-1}$) - Figure (9c, d)

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. Figure 9-c shows dislocation cells and dislocation tangles can be seen in Figure 9-d. This microstructure is again consistent with observations of the beginning of the third stage of work hardening. In the same manner, the detailed internal structure of dislocation cell boundaries consists of arrays of wavy dislocations, as shown in Figure 9-d.

III.4 Microstructural comparison

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.

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

Single crystal vs. polycrystal – static and dynamic deformation. The detailed microstructural study indicates that the resulting microstructure of single 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 β factors (Figure 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 quite expectable and natural.

IV. DISCUSSION and SUMMARY

This work represents an attempt to investigate and characterize the thermomechanical response of high purity copper, in the single and polycrystalline form. 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 quite central in understanding the results presented in this work.

Before discussing and summarizing the main results of this work, it should be reminded 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 to the global single-crystal response for 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) make no exception.

The main issue here is the 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 β_{ave} 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 of β_{int}=0.9 falls relatively far off what was measured here for the 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 infrared detectors, which does not detract from the pioneering character of their work.

It was observed that the single and polycrystalline copper specimens are characterized by different β_{ave}. In spite of this difference, Figure 4 reveals a very similar dependence of β_{ave} on the strain rate, noting that the relationship is rather 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 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 β_{ave} values than the 2 orientations tested for the single crystals. 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 comprise 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 β values. Therefore, one could tentatively rationalize the different behaviors of Ta and Cu by invoking twinning in the polycrystalline Ta at high strain-rates, which in any case calls for additional thermomechanical studies with in-depth microstructural characterization.

Back to Cu, one should note that in the quasi-static regime, there seems to be a break of the linear $\beta_{ave} - \dot{\varepsilon}$ relationship at least for the single crystals, and also perhaps for the polycrystalline copper, at low strain-rates as evidenced by comparing Figures 4(a) and (b). Note that the β_{ave} values measured for the single crystal show a relatively good agreement with those calculated from discrete dislocation plasticity by Benzerga et al. [8]. The natural question which arises here relates to whether the rapid quasi-static tests can be considered as adiabatic. To address this issue, one may refer to Rabin and Rittel's [27] analysis of the temperature gradient in cylindrical specimens subjected to a 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 that $\alpha = 1.12x10^{-4} m^2 / s$ (thermal conductivity), $R = 3mm$ (specimen's radius), and a time

lapse of $0.5s \le t \le 5s$, one obtains that the corresponding Fourier number is in the range $6.3 \le Fo \le 63$. 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 inferior to 5%. In such a case, the heat convection has almost no effect on the temperature distribution, which in turn suggests that the test can be considered as adiabatic (negligible $k\nabla^2 T$).

Considering now the storage of energy of cold work, the microstructural characterization was precisely 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 β factors, all the investigated specimens exhibit an apparently highly similar microstructure, whether single 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 only to 25%, as compared to 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, when compared to 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 2 materials, and the *grain boundaries* present in the polycrystal only. The reported microstructural resemblance refers obviously to the bulk material only, 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 and the 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 Figure 7, a first estimate shows that the polycrystal stores roughly twice as much energy of cold work than the single crystal does. 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/sinks for dislocations, as a result of plastic incompatibility between grains. The partition of stored energy into two terms, one being the bulk storage (single crystal) and the second being identified as the grain boundaries contribution has not been quantified in previous work to the best of our knowledge.

One can thus summarize this work as a joint thermomechanical-microstructural study of the thermomechanics of copper which fist show 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 β_{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 and polycrystalline), the stored energy of cold work 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 dependence on the strain rate. Within a given group, the resemblance is expected due to the lack of dependence on the strain rate. Between the two groups, the strong microstructural resemblance coupled to the different capability of energy storage can be ascribed to the presence of grain-boundaries in the polycrystalline samples.

V. CONCLUSIONS

A systematic comparative study was carried out on the thermomechanical response and properties of single and polycrystalline high purity copper. The following conclusions can be drawn from this work:

1. The mechanical response of each class is both very different in terms of strain-hardening, although both are distinctly strain-rate sensitive.

2. A simplified interpretation of the Taylor-Quinney coefficient (β_{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 stored energy of cold work 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. 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 higher level of storage of energy of cold work by the polycrystalline copper is due to the presence of grain-boundaries in this group.

6. It is therefore suggested to carry out similar studies on other materials to pinpoint the individual contribution of the bulk material and the grain boundaries on the overall process of energy storage.

ACKNOWLEDGEMENT

The research support provided by the Caltech Center for the Predictive Modeling and Simulation of High-Energy Density Dynamic Response of Materials through the U.S. Department of Energy contract DE-FC52-08NA28613 is gratefully acknowledged.

REFERENCES

[1] Bever M, Holt D, Titchener A. The Stored Energy of Cold Work. London: Pergamon Press, 1973.

[2] Kolsky H. An investigation of the mechanical properties of materials at very high rates of loading. Proc. Phys. Soc. London 1949;62-B:676.

[3] Marchand A, Duffy J. An experimental study of the formation process of adiabatic shear bands in a structural steel. J. Mech. Phys. Solids 1988;36:251.

[4] Boley BA, Weiner JH. Theory of Thermal Stresses. New York, NY: J. Wiley and Sons, 1960.

[5] Rittel D. The conversion of plastic work to heat during high strain rate deformation of glassy polymers. Mechanics of Materials 1999;31:131.

[6] Rittel D, Landau P, Venkert A. Dynamic recrystallization as a potential cause for adiabatic shear failure. Physical Review Letters 2008;101:165501.

[7] Rittel D, Wang ZG, Merzer M. Adiabatic shear failure and dynamic stored energy of cold work. Physical Review Letters 2006;96:075502.

[8] Benzerga A, Brechet Y, Needleman A, Van der Giessen E. The stored energy of cold work: Predictions from discrete dislocation plasticity. Acta Mater. 2005;53:4765.

[9] Longere P, Dragon A. Evaluation of the inelastic heat fraction in the context of microstructure-supported dynamic plasticity modelling. Intl. J. Impact Engng. 2008;35:992.

[10] Mason JJ, Rosakis AJ, Ravichandran G. On the strain and strain rate dependence of the fraction of plastic work converted into heat: an experimental study using high speed infrared detectors and the Kolsky bar. Mechanics of Materials 1994;17:135.

[11] Hodowany J, Ravichandran G, Rosakis AJ, Rosakis P. Partition of plastic work into heat and stored energy in metals. Exp. Mech. 2000;40:113.

[12] Rosakis P, Rosakis AJ, Ravichandran G, Hodowany JA. Thermodynamic internal variable model for the partition of plastic work into heat and stored energy in metals. J. Mech. Phys. Solids 2000;48:581.

[13] Stainier L, Ortiz M. Study and validation of a variational theory of thermo-mechanical coupling in finite visco-plasticity Int. J. Solids and Structures 2010;47:705.

[14] Kapoor R, Nemat-Nasser S. Determination of temperature rise during high strain rate deformation. Mechanics of Materials 1998;27:1.

[15] Taylor GI, Quinney H. The latent energy remaining in a metal after cold working. Proc. Royal Soc. London 1934;143:307.

[16] Farren WS, Taylor GI. The heat developed during plastic extension of metals. Proc. R. Soc. 1925;A107:422.

[17] Rittel D, Silva ML, Poon B, Ravichandran G. Thermomechanical behavior of single crystalline tantalum in the static and dynamic regime. Mechanics of Materials 2009;41:1323.

[18] Hartley KA, Duffy J, Hawley RH. Measurement of the temperature profile during shear band formation in mild steels deforming at high-strain rates. J. Mech. Phys. Solids 1987;35:283.

[19] Rittel D, Bhattacharyya A, Poon B, Zhao J, Ravichandran G. Thermomechanical characterization of pure polycrystalline tantalum. Matls. Sc. and Engng. A 2007;A447:65.

[20] Regev A, Rittel D. Simultaneous transient temperature sensing of impacted polymers using infrared detectors and thermocouples. Exp. Mech. 2008;48:675.

[21] Nemat-Nasser S, Ni LQ, Okinaka T. A constitutive model for fcc crystals with application to polycrystalline OFHC copper. Mechanics of Materials 1998;30:325.

[22] Rittel D, Lee S, Ravichandran G. Large strain constitutive behavior of OFHC copper over a wide range of strain-rates using the shear compression specimen. Mechanics of Materials 2002;34:627.

[23] Follansbee PS, Kocks UF. A constitutive description of the deformation of copper based on the use of the mechanical treshold stress as an internal state variable. Acta Metall 1988;36:81.

[24] Landau P, Shneck RZ, Makov G, Venkert A. Microstructure evolution in deformed copper. J. Matls. Sc. 2007;42:9775.

[25] Armstrong RW, Zerilli FJ. High rate straining of tantalum and copper. J. Phys. D.: Appl. Phys. 2010;43.

[26] Padilla HA, Smith CD, Lambros J, Beaudoin AJ, Robertson IM. Effects of deformation twinning on energy dissipation in high rate deformed zirconium. Metallurgical and Material Transactions A 2007;38A:2916.

[27] Rabin Y, Rittel D. Infrared temperature sensing of mechanically loaded specimens: thermal analysis. Experimental Mechanics 2000;40:197.

[28] Molinari A, Ravichandran G. Constitutive modeling of high-strain-rate deformation in metals based on the evolution of an effective microstructural length Mechanics of Materials 2005;37:737.

[29] Landau P, Makov G, Shneck RZ, Venkert A. Universal strain - temperature dependence of dislocation structure evolution in FCC metals. Acta Materialia 2011;59:5342.

FIGURES

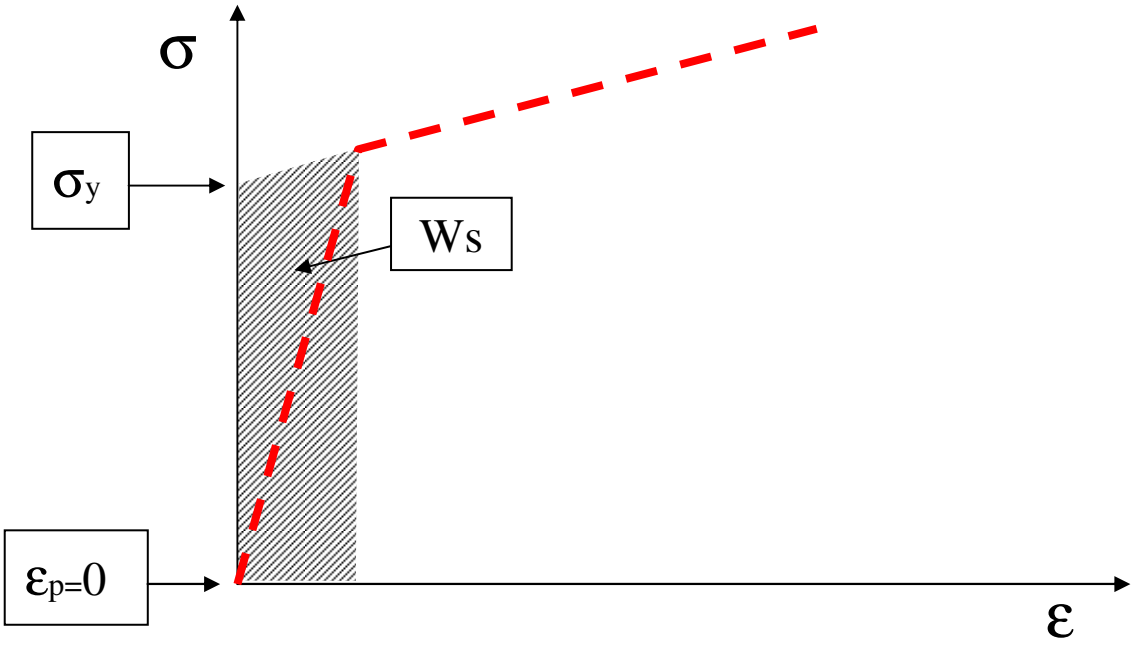

Figure 1: Schematic representation of the correction brought to the estimation of the strain energy density. The dashed line is the stress-strain curve obtained from a dynamic test, for which the initial elastic slope is incorrect. The flow stress is extrapolated to intercept the stress axis at ε=0, which is *approximated* as zero plastic strain.

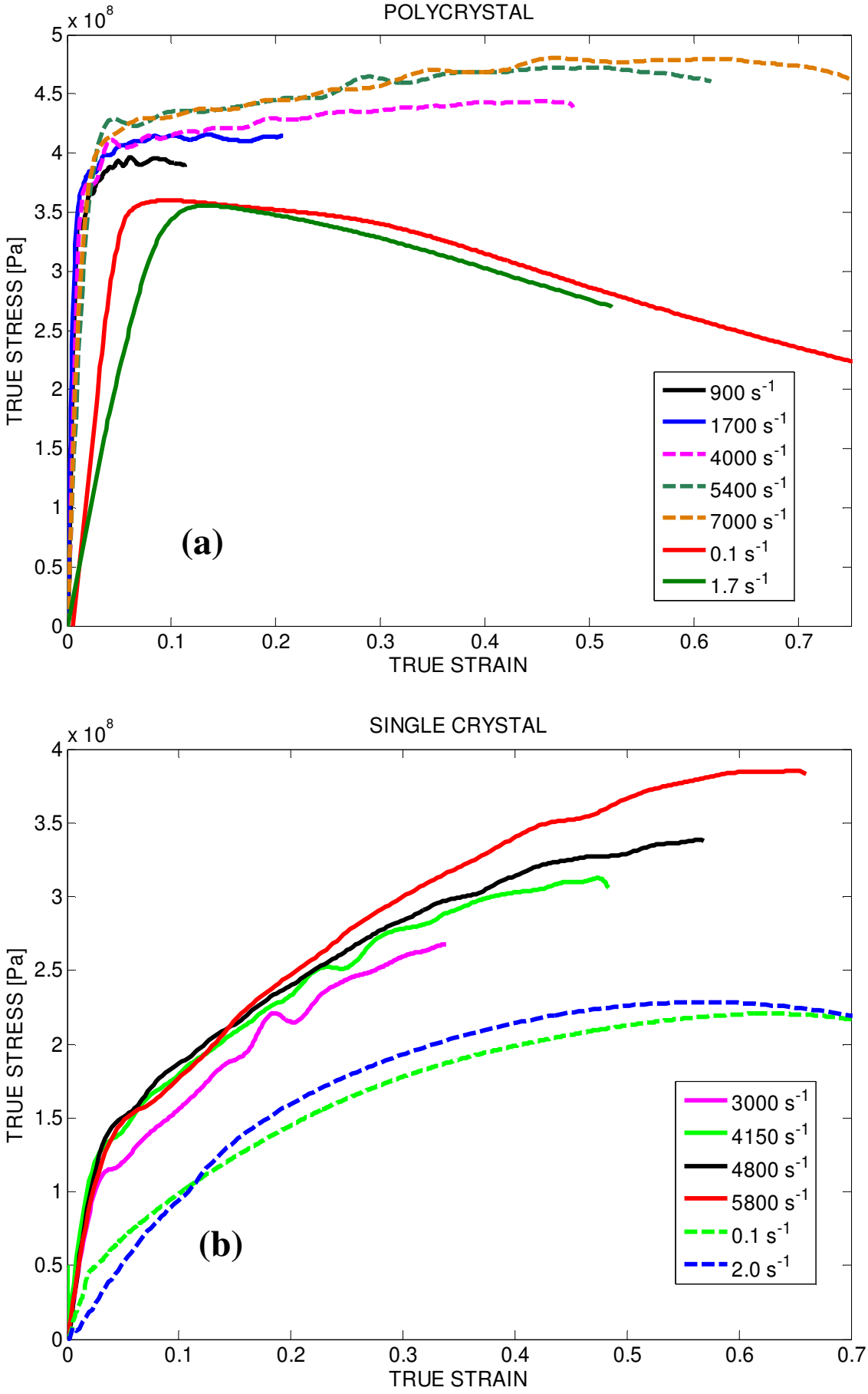

Figure 2: True stress-strain curves for (a) polycrystalline and (b) single crystal copper at various strain rates

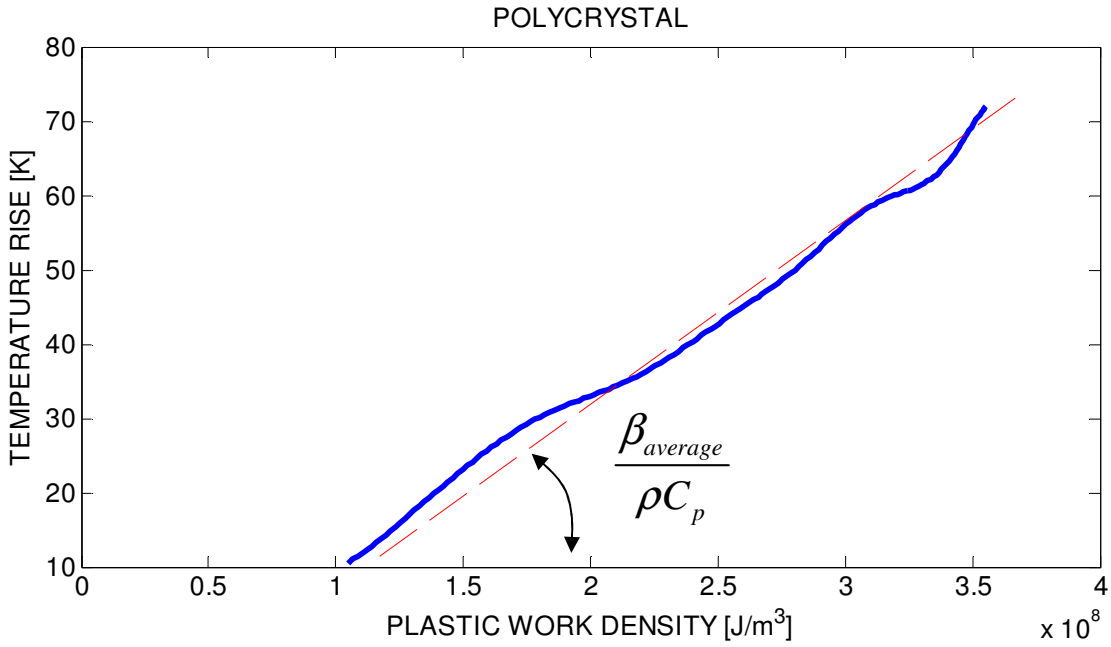

Figure 3: Typical plot of the temperature rise as a function of the plastic work density. Note that the slope of the curve corresponds to the average value of β_{int}.

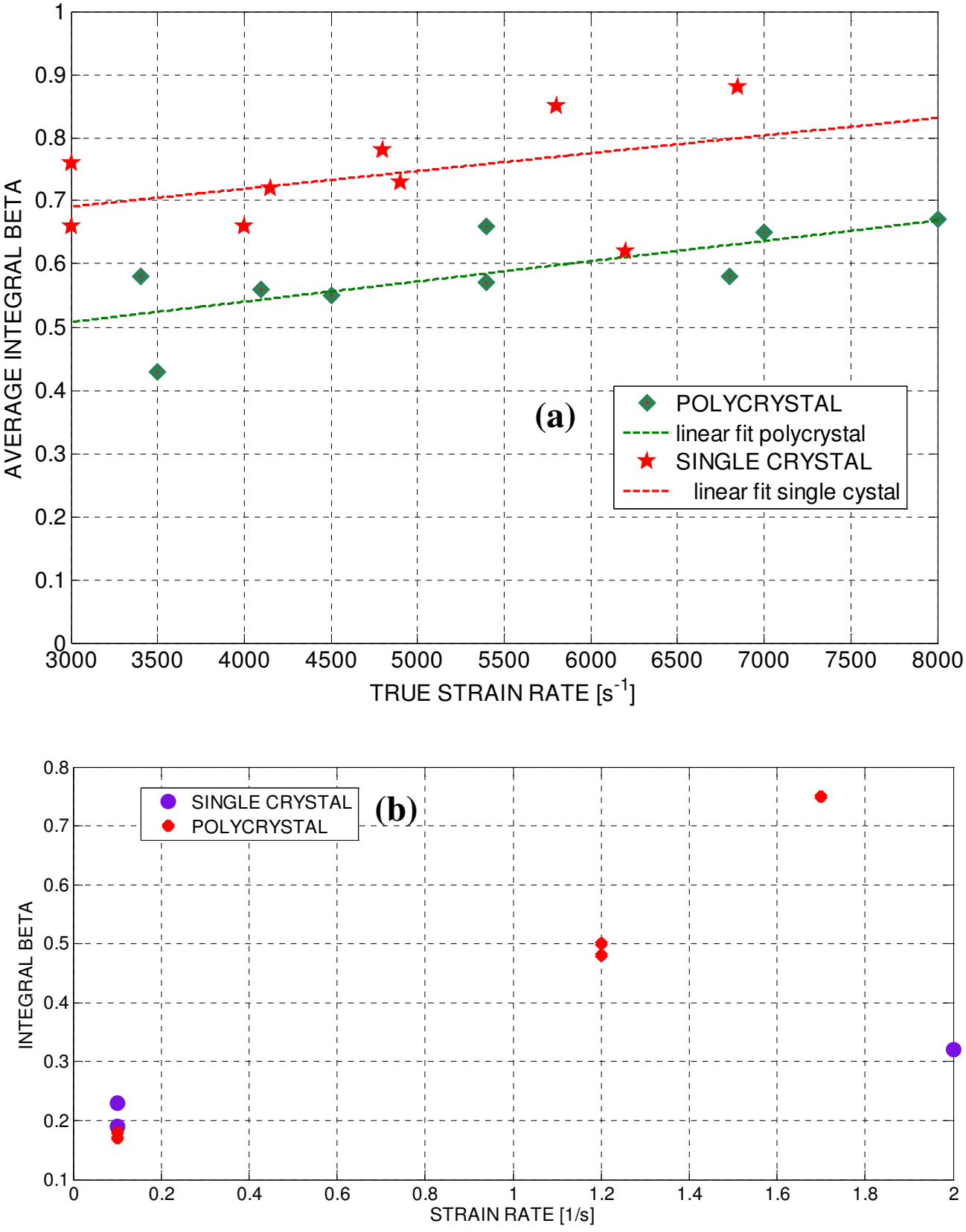

Figure 4: Measured values of $\beta_{ave.}$ for single and polycrystalline copper as a function of the strain-rate, (a) in the dynamic and (b) quasi-static regime.

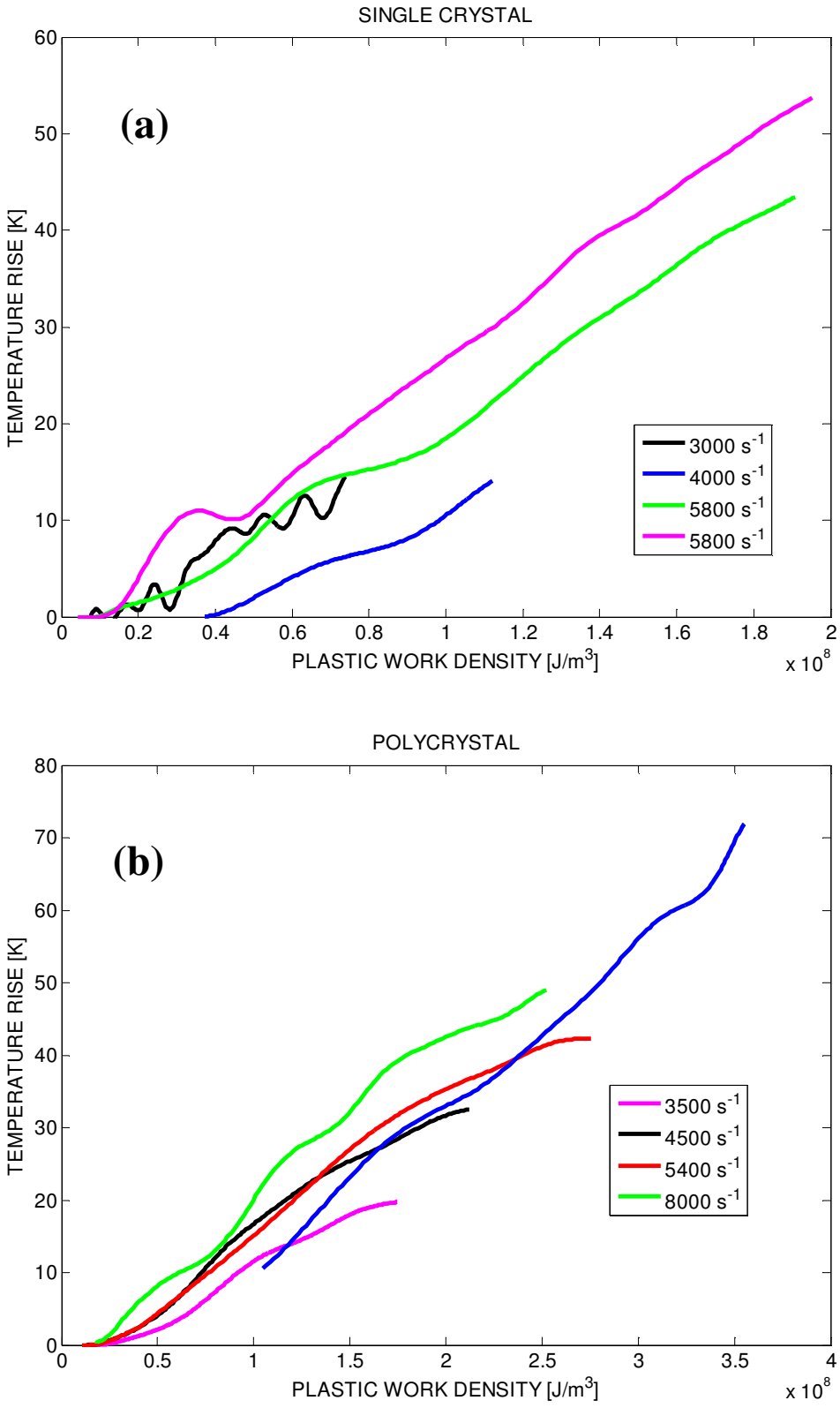

Figure 5: Evolution of the temperature as a function of the plastic work density in the dynamic regime, for (a) single and (b) polycrystalline copper.

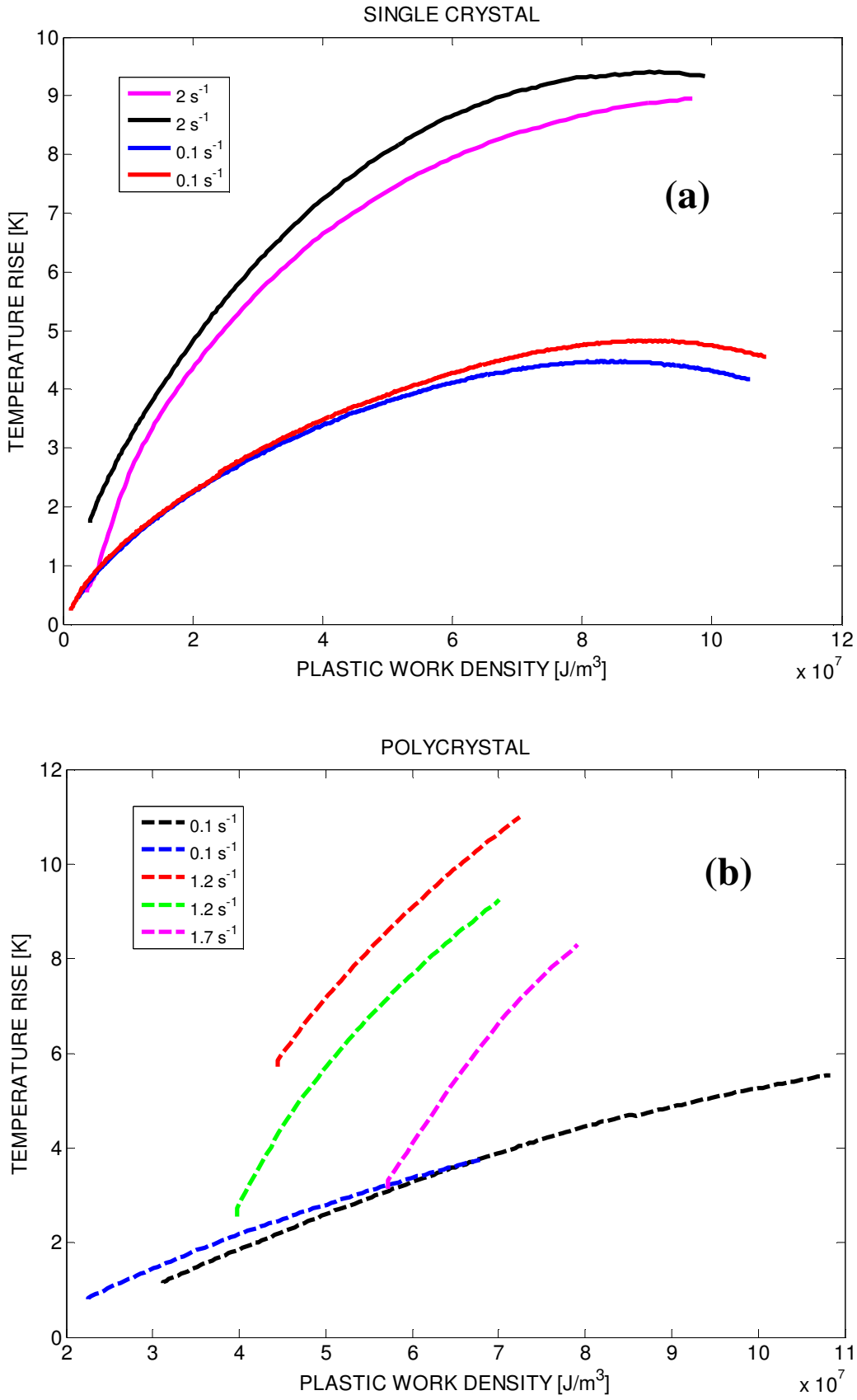

Figure 6: Evolution of the temperature as a function of the plastic work density in the static regime, for (a) single and (b) polycrystalline copper.

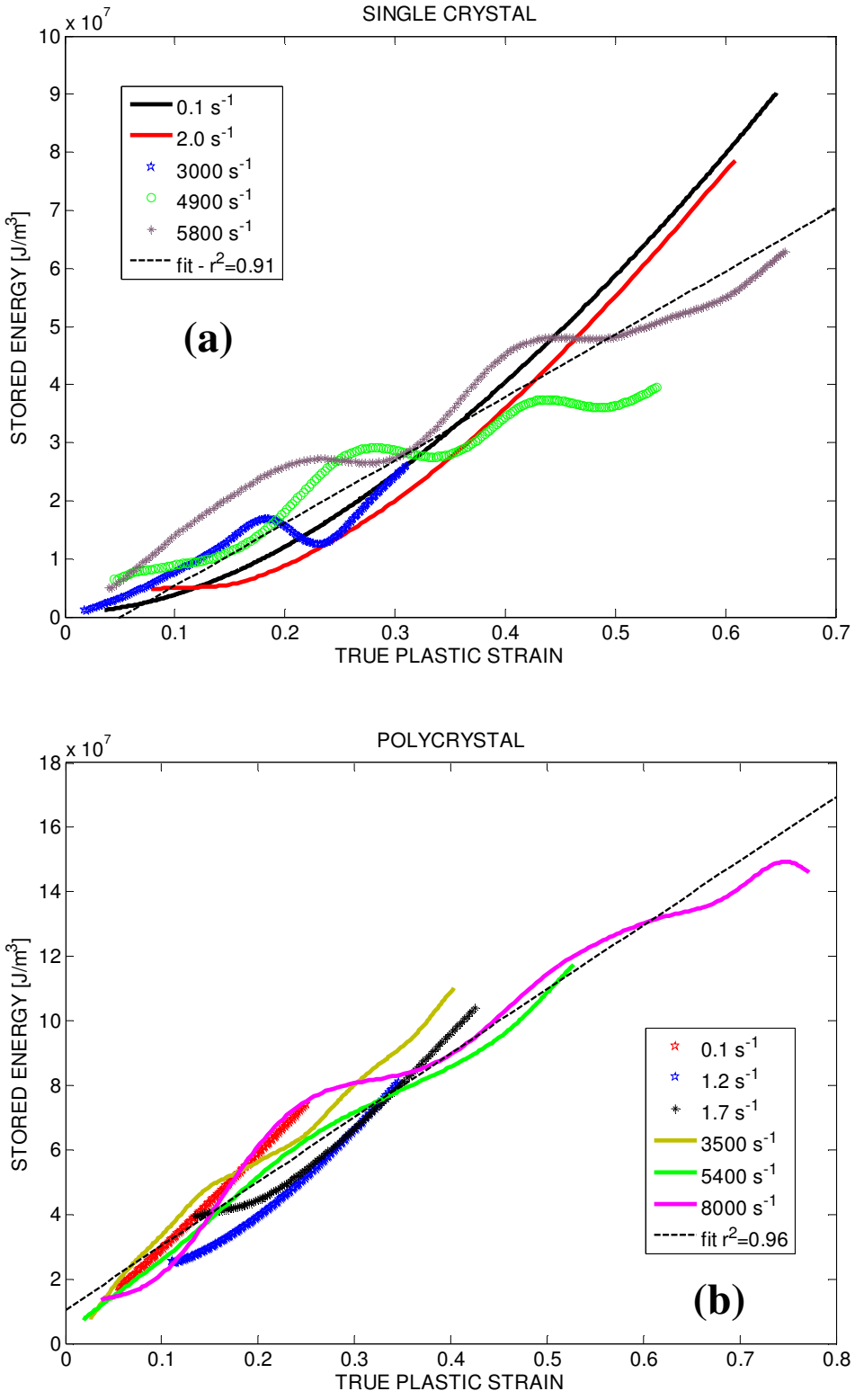

Figure 7: Stored energy density as a function of plastic strain in (a) single crystalline Cu and (b) polycrystalline Cu, at various strain rates. Trendlines (dashed) correspond to linear best-fits.

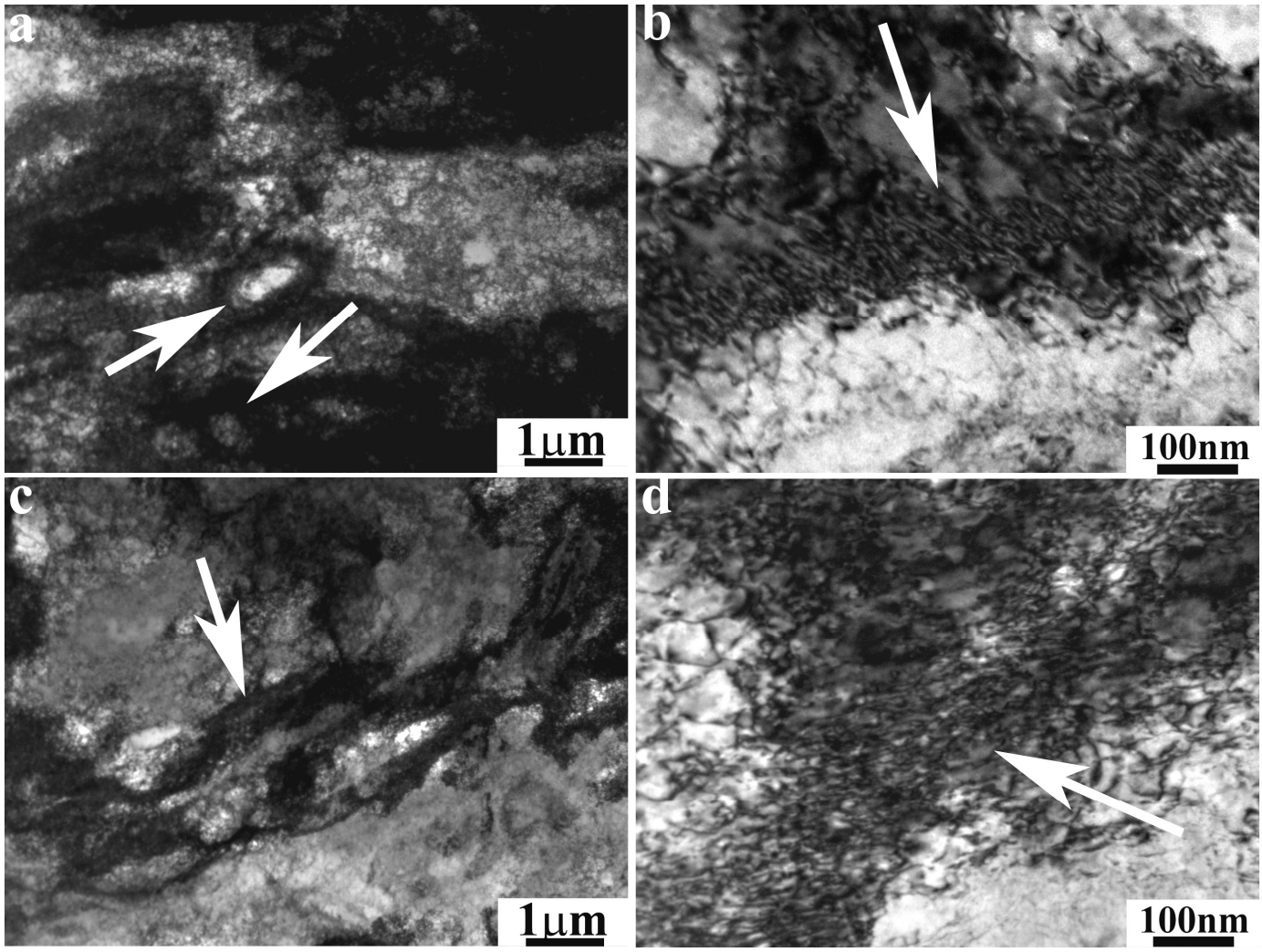

Figure 8: TEM micrographs of single crystals deformed to 50%: a- quasi-static: low magnification image of dislocation cells (arrowed) and tangles. b- quasi-static: high magnification of the detailed wavy arrangement of dislocations (arrowed) within the cells boundaries. c- dynamic: low magnification view of dislocation cells (arrowed). d- dynamic- high magnification of the detailed structure consisting of wavy dislocations (arrowed).

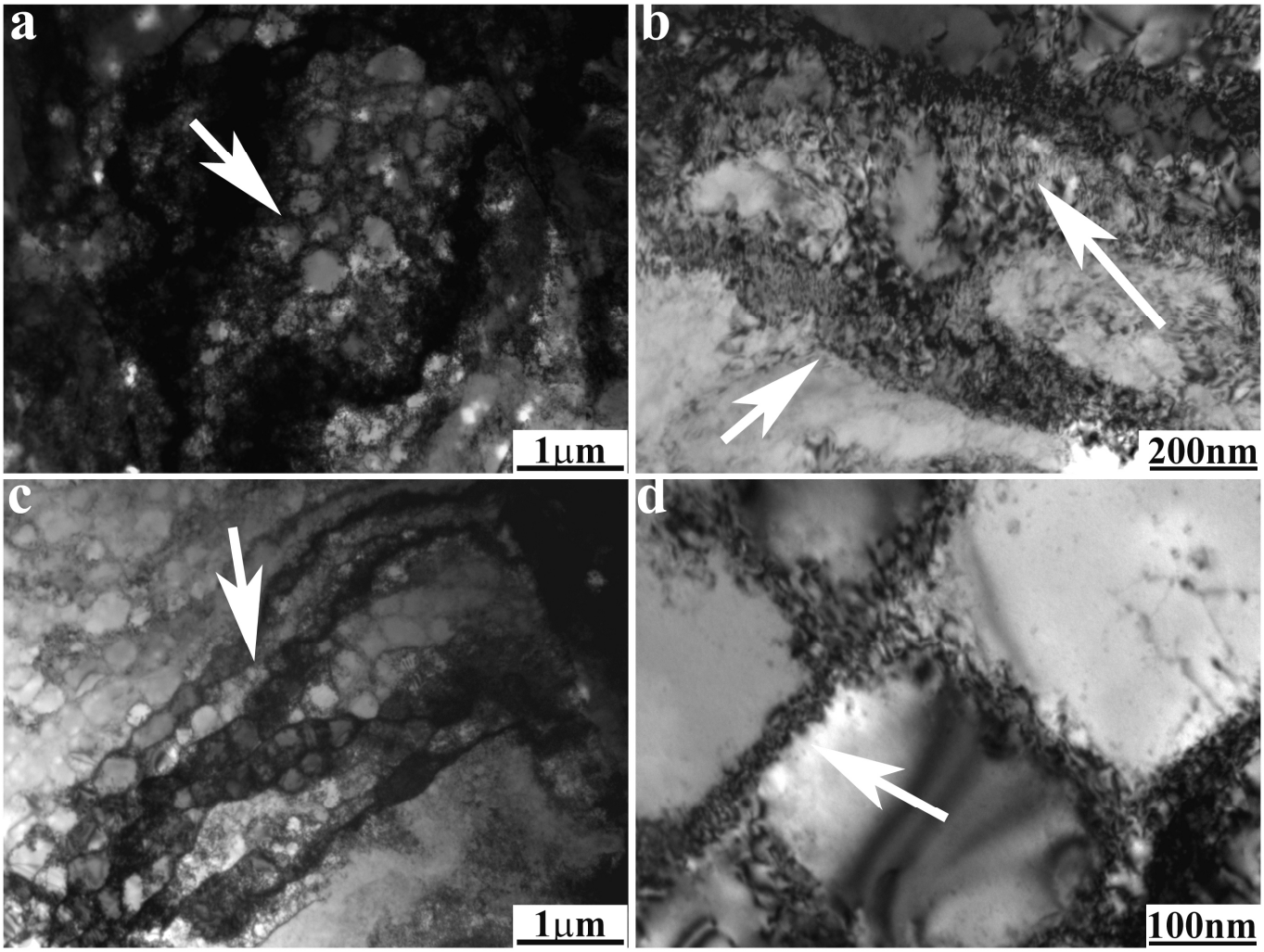

Figure 9: TEM micrographs of polycrystals deformed to 25%: a- quasi-static: low magnification image of dislocation cells (arrowed) and tangles. b- quasi-static: high magnification of the detailed wavy arrangement of dislocations (arrowed) within the cells boundaries. c- dynamic: low magnification view of dislocation cells (arrowed). d- dynamic- high magnification of the detailed structure consisting of wavy dislocations (arrowed).