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THERMODYNAMIC ANALYSIS OF ENERGY STORAGE RATE DURING UNIAXIAL TENSILE DEFORMATION OF POLYCRYSTALLINE METAL

TERMODYNAMICZNA ANALIZA POJĘCIA ZDOLNOŚCI MAGAZYNOWANIA ENERGII W PROCESIE JEDNOOSIOWEGO ROZCIĄGANIA POLIKRYSTAŁU

The stored energy e_s due to plastic deformation is defined as the change in internal energy measured at stress free state of material, and it characterises the cold-worked state. Both cold-worked state and the stored energy at each instant of deformation depend on the deformation history. Therefore, the instantaneous rate de_s/dw_p of energy storage seems to be an appropriate measure of the energy conversion process (w_p is the work of plastic deformation). The rate of energy storage is important characteristic of the whole energy storage processes. It is a macroscopic quantity that is influenced by many microscopic mechanisms. Each of them is described by the separate internal parameter H_i .

In mathematical description, the stored energy is a function of $H_1, H_2, H_3, \dots, H_n$. Since there exist couplings between different mechanisms the function can not be, in general, written in the form: $\sum_{i=1}^n e_s^{(i)}(H_i)$. The similar remark concerns also the energy storage rate.

The present paper is devoted an answer if it is possible to distinguish the influence of the change in given internal parameter on the rate of energy storage.

In order to find the answer the theoretical analysis of energy storage rate on the basis of phenomenological thermodynamics of plastic deformation was done. The theoretical description of the experimental method of stored energy determination is presented. The results of the analysis have been used to support the additive partitioning of the resultant rate of the energy stored and to show experiment which allows distinguishing the particular components. Each component represents the specific microscopic mechanism.

The analysis of preliminary experimental data arrived at the conclusion that in the initial stage of plastic deformation of polycrystalline metal at least two components of the energy

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storage rate exist. One of them is associated with the rise of dislocation density, and another one is related to the internal stress field due to elastic accommodation of incompatible strains in the vicinity of grain boundaries.

Energia zmagazynowana została zdefiniowana jako przyrost energii wewnętrznej badanego materiału, wywołany odkształceniem plastycznym i wyznaczony w stanie odciążonym. Charakteryzuje ona stan odkształconego materiału. Ten stan a więc i energia zmagazynowana zależy od historii odkształcenia. Miarą przemiany energii w danym punkcie procesu deformacji jest stosunek nieskończenie małej zmiany energii zmagazynowanej de_s do nieskończenie małego przyrostu pracy odkształcenia plastycznego dw_p odpowiadającego tej zmianie. Tę wielkość nazwano zdolnością magazynowania energii. Zdolność magazynowania energii $\frac{de_s}{dw_p}$ jest makroskopowym przejawem wielu mikroskopowych mechanizmów. Każdemu z nich przypisano parametr H_i .

Energię zmagazynowaną można przedstawić jako funkcję parametrów: $H_1, H_2, H_3, \dots, H_n$. Między tymi parametrami występują sprzężenia i dlatego, w ogólnym wypadku, funkcji $e_s(H_1, H_2, H_3, \dots, H_n)$ nie można zapisać w formie: $\sum_{i=1}^n e_s^{(i)}(H_i)$.

Powstaje pytanie, czy zdolność magazynowania energii można przedstawić jako sumę składników, odpowiadających poszczególnym parametrom H_i . Odpowiedź na nie jest głównym celem niniejszej pracy. Uzyskano ją drogą teoretycznej analizy zdolności magazynowania energii na gruncie fenomenologicznej termodynamiki odkształcenia plastycznego. W związku z tym przedstawiono w skrócie teoretyczny opis eksperymentalnej metody wyznaczania energii zmagazynowanej.

Wynik analizy teoretycznej posłużył do zaproponowania eksperymentów umożliwiających rozróżnienie i identyfikację niektórych składników zdolności magazynowania energii.

Ze wstępnych danych doświadczalnych wynika, że na początku odkształcenia plastycznego polikryształu występują co najmniej dwa składniki zdolności magazynowania energii. Jeden z nich jest związany ze wzrostem gęstości dyslokacji, drugi — odpowiada generacji pola naprężeń wewnętrznych, wywołanej sprężystą akomodacją niekompatybilnych odkształceń poszczególnych ziaren polikryształu.

1. Introduction

When metals deform plastically an energy conversion occurs; a part of the mechanical work w_p done during the single cycle of plastic straining is converted into the heat q_c . The rest of it remains in the metal and it is known as the stored energy e_s .

The energy storage process in metals was discovered by Taylor and Quinney [1]. It remains the subject a large number of experimental [2–6] and theoretical studies [7–9]. It is usually characterised by the dependence of e_s on w_p or strain ϵ .

The stored energy describes the cold-worked state and it represents the change in internal energy measured at external stress free state of a tested metal.

$$e_s = w_p - q_c. \quad (1)$$

Both cold-worked state and the stored energy at each instant of deformation depend on the deformation history. Therefore, the instantaneous rate of energy storage (de_s/dw_p) seems to be an appropriate measure of the energy conversion process. The rate of energy

storage is important characteristic of the whole energy storage process. It is a macroscopic quantity that is influenced by many micro-scale mechanisms.

The rate de_s/dw_p can be found by differentiating e_s as a function w_p provided that the function is determined without interruption of the deformation process. The experimental method of stored energy determination employed in present work enables application of such technique [10]. In the present paper thermodynamic description of the method is briefly presented.

It has been shown experimentally, that in the initial stage of plastic deformation of polycrystalline metals, the dependence of the de_s/dw_p ratio on the work w_p expended during plastic deformation has a maximum [1].

The physical phenomena responsible for occurrence of the maximum were discussed in [12–14]. The growth in the rate of energy storage in initial stage of plastic deformation is associated with an increase of dislocation density and with internal stresses caused by elastic accommodation of incompatible deformations of neighbouring grains. In a polycrystalline metal the slip in individual grains leads to the change of the shape of the grains. This aspect of the slip appears in the form of relief on the free surface of the specimen, where grains have random orientation to the applied stress [14, 15]. However in order to preserve the material continuity during straining some components of the micro-strain field are forbidden, and as the result the additional micro-stresses are generated. This effect is called elastic accommodation and the additional micro-stresses are termed accommodation stresses [15, 16].

It has been shown, that maximum of energy storage rate is closely related to the change in the mode of a slip. This maximum is a macroscopic manifestation of the change of the deformation mode from a homogeneous multi-system slip into micro shear banding [13, 14]. Thus de_s/dw_p is important macroscopic quantity that depends on number of internal parameters H describing micro-scale mechanisms. Each mechanism is described by the separate internal parameter H_i .

In mathematical description, the stored energy is a function of $H_1, H_2, H_3, \dots, H_n$. Since there exist couplings between different mechanisms the function can not be, in

general, written in the form: $\sum_{i=1}^n e_s^{(i)}(H_i)$. The similar remark concerns also the energy storage rate.

The question appears: Is it possible to distinguish the influence of particular microscopic mechanism on the rate of energy storage? In the other words, is it possible to distinguish the influence of the change in given internal parameter on the rate of energy storage? In order to find the answer, the theoretical analysis of energy storage rate, on the basis of phenomenological thermodynamics of plastic deformation is needed. Such kind of analysis is the main aim of the present work. The results of the analysis have been used to support the additive partitioning of the resultant rate of energy stored and to show experiment which allows distinguishing the particular components of the energy storage rate.

2. Thermodynamic description of the experimental method of stored energy determination

For description of the thermodynamic state of tested specimen, the following set of independent parameters is adopted:

$$Y^{Tp} = \{T, p_\alpha, \mathbf{H}\}, \quad (2)$$

where T is the temperature of the specimen, p_α is the generalised stress work conjugated with elastic strain ε_α^E , H_i ($i = 1 \dots n$) is the number of internal parameters, describing of microstructure evolution.

The thermodynamic potential, whose natural variables are the chosen parameters, is the Gibbs function.

Using first law of thermodynamics, the thermal equation of state resulted from the Gibbs function [17] for the entropy as well as, assuming that deformation process is homogeneous and quasistatic the following simplified equation for the temperature of the specimen is obtained [18]:

$$c_p dT = \bar{d}w_p - de_s(\mathbf{H}) - \frac{T}{\rho_0} \alpha_\beta dp_\beta + \bar{d}q. \quad (3)$$

Here w_p is the work of plastic deformation and q is defined by formula: $\int dq = -q_c$, where q_c is the heat transferred to the surroundings when the specimen is unloaded and its temperature came back to initial one. The quantities w_p and q represent energies per mass unit. It was assumed that the specific heat c_p and the coefficient of linear thermal expansion α_β of tested material are independent of \mathbf{H} . The sign α is introduced for notation of increments that are not total differentials.

At uniaxial tensile deformation the only non-zero component of Cauchy stress tensor is $\sigma = \sigma_{11} = P(t)/A(t)$, where $P(t)$ is instantaneous force of tensile, $A(t)$ is instantaneous cross-section area of a specimen. The incremental work done on the gauge part of the specimen is:

$$\bar{d}w = \frac{1}{\rho} \sigma d\varepsilon, \quad (4)$$

where ρ is instantaneous mass density of the specimen.

The axial component of elastic strain tensor ε_{11}^E is defined as

$$\varepsilon_{11}^E \equiv \varepsilon^E = \ln \frac{l(t)}{l^*(t)}, \quad (5)$$

where $l^*(t)$ is the gauge length of the specimen in the instantaneous unloaded configuration.

If the specimen was deformed only plastically ($l^* = \text{constans}$), then we would have:

$$\bar{d}w = dw_E = \frac{1}{\rho} \sigma d\varepsilon = \frac{1}{\rho_0} \tau d\varepsilon^E; \quad \tau = \frac{\rho_0}{\rho(t)} \sigma. \quad (6)$$

The stress τ is known as Kirchhoff stress. Note that in contrary to σ the τ stress is independent of the current cross-section area of the test specimen.

$$d\varepsilon = \frac{dl}{l} = d\varepsilon^E + d\varepsilon^p, \text{ then from (5) } \varepsilon_p = \ln \frac{l^*(t)}{l_0}. \quad (7)$$

This property implies the additive decomposition of dw :

$$\bar{d}w_p = \bar{d}w - \bar{d}w_E = \frac{1}{\rho_0} \tau d\varepsilon^p. \quad (8)$$

Under uniaxial deformation the simplified equation for the temperature takes the form:

$$c_p(T) dT = \bar{d}w_p - de_s(H) - \frac{T}{\rho_0} \alpha d\tau + \bar{d}q, \quad (9)$$

where we have assumed that c_p is independent of the stress.

The equation (9) is used as a basis for the development of the experimental method of measurement of $e_s(H)$ during uniaxial tensile deformation.

Let us heat the unloaded specimen by means of controlled supply of electric power $r(t_1)$. In such case, the formula for temperature of the heated specimen is as follows:

$$c_p(T') dT' = r(t_1) dt_1 + \bar{d}q'. \quad (10)$$

If the specimen is heated in such a way that the temperature increase with time t_1 during the heating is identical with that measured during tensile loading and the straining and the electric heating are performed under identical conditions, then

$$c_p(T) dT = c_p(T') dT'; \quad \bar{d}q = \bar{d}q' \text{ thus } r(t_1) dt_1 = \bar{d}w_p - de_s(H) - \frac{T}{\rho_0} \alpha d\tau. \quad (11)$$

The temperature distribution on the specimen surface is determined through measurement of IR radiation power emitted by the strained specimen.

Integration of (11)₃ gives

$$e_s = w_p - \int_0^t r(t_1) dt_1 - \frac{1}{\rho_0} \int_0^t \alpha T d\tau; \quad w_p = \int_0^t \bar{d}w_p.$$

Since the temperature variations are small the αT term can be approximated by constant value αT_0 where T_0 is the reference temperature. Then the above equation becomes

$$e_s = w_p - q_c - \frac{\alpha}{\rho_0} T_0 \tau, \quad q_c = \int_0^t r(t_1) dt_1. \quad (12)$$

The instantaneous value of w_p is determined from the force versus elongation plot recorded during tensile deformation (Fig. 1). The heat q_c transferred to surroundings is obtained from the measurement of the electrical power $r(t_1)$, and equation (12)₁ enables

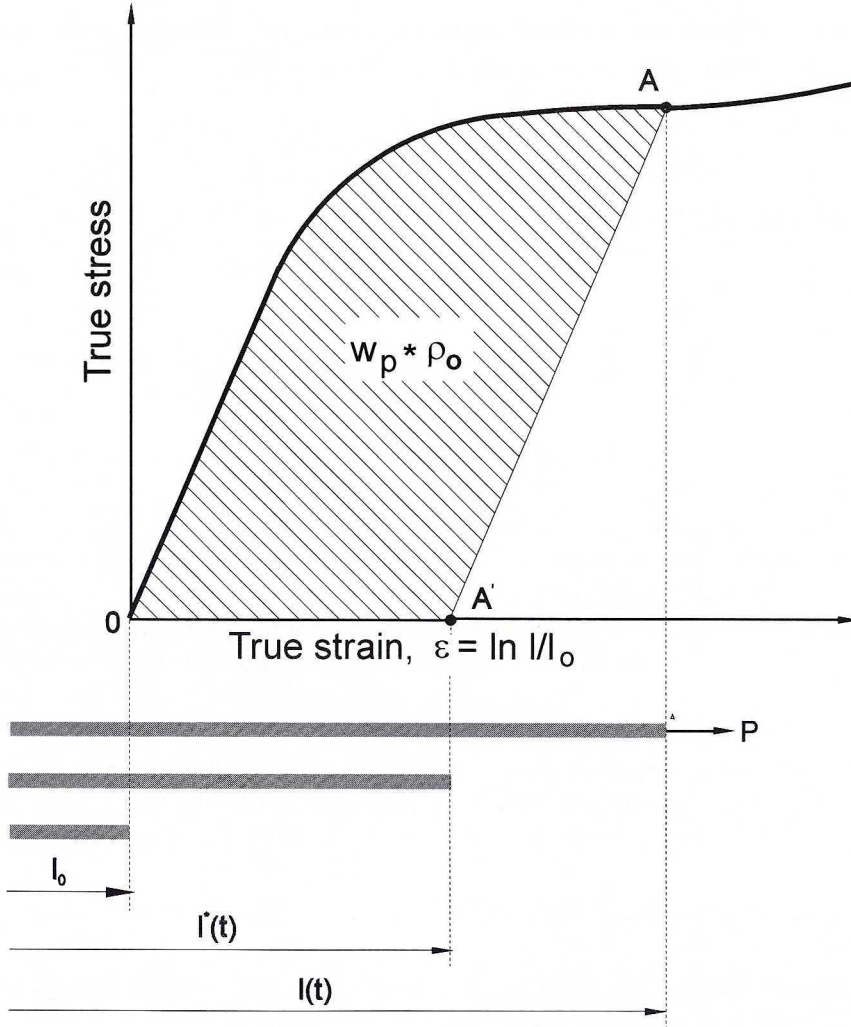


Fig. 1. Determination of the plastic deformation work

experimental determination of stored energy e_s . Under condition of homogeneous deformation, the method makes possible to measure in situ the stored energy without use of a calorimeter and without interrupting deformation process.

3. The energy storage rate

In the course of loading $\varepsilon^p(t)$ is a monotonic function of time t . Hence, the time t can be replaced by the plastic strain ε^p . In effect, all internal parameters H (independently of their physical meaning) are some functions of ε^p .

$$\mathbf{H} = \mathbf{H}(\varepsilon^p). \quad (13)$$

The difference between incremental plastic work and energy storage can be presented in the form:

$$\bar{d}w_p - de_s(H) = \bar{d}w_p(1 - Z), \quad (14)$$

$Z = \frac{de_s(H)}{dw_p}$, where Z is the quantity describing energy conversion at a given instant of deformation.

For infinitesimal increment of stored energy: $de_s(H) = \sum_{i=1}^n \left(\frac{\partial e_s}{\partial H_i} \right) dH_i$.

Taking into consideration that \mathbf{H} is function of ε^p and $\bar{d}w_p = \frac{1}{\rho_0} \tau d\varepsilon_p$, the instantaneous rate of energy storage Z , during uniaxial tensile deformation, can be written in the form:

$$Z = \frac{de_s}{dw_p} = \frac{\rho_0}{\tau} \frac{de_s}{d\varepsilon^p} = \frac{\rho_0}{\tau} \cdot \sum_{i=1}^{i=n} \frac{\partial e_s(H)}{\partial H_i} \cdot \frac{dH_i}{d\varepsilon^p}. \quad (15)$$

From (15) it follows that the rate of energy storage is a sum of particular components. Each of them describes the contribution of some internal mechanism (that is represented by H_i) to the energy conversion.

$$Z = \sum_{i=1}^n A_i(\varepsilon^p) \frac{dH_i}{d\varepsilon^p}, \quad \text{where} \quad A_i = \frac{\rho_0}{\tau} \frac{\partial e_s(H)}{\partial H_i}. \quad (16)$$

4. Experiments

The experiments on an austenitic stainless steel were performed. The composition of the steel is: 0.05 wt.% C, 1.35 wt.% Mn, 1.0 wt.% Si, 0.016 wt.% P, 0.008 wt.% S, 18.58 wt.% Cr, 17.3 wt.% Ni, 0.025 wt.% W, 0.02 wt.% Mo, 0.04 wt.% Cu, 0.03 wt.% V, 0.013 wt.% Ti and the balance Fe. Cold-rolled strips with a cross-section of 25 mm × 4 mm were initially annealed at 1050°C, water quenched and 50% cold rolled. The tensile specimens were machined from the material prepared in this way (Fig. 2).

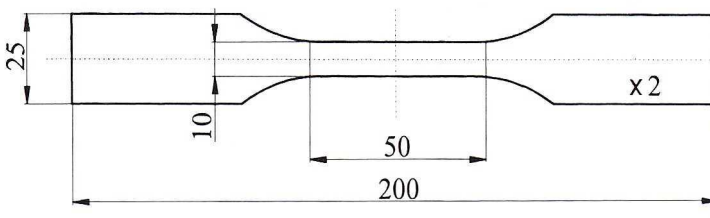


Fig. 2. Shape of the specimen

Specimens were divided into two groups. The first group (group A) for 1h at 950° was annealed and water quenched. It have been produced a homogeneous microstructure with a grain size $\approx 8 \mu\text{m}$. The specimens of the second group (B) were annealed for 2h at 1100°C and water quenched producing a homogeneous microstructure with grain size $\approx 80 \mu\text{m}$.

All specimens were strained in tensile tests carried out on a testing machine, with the constant rate $\dot{\epsilon} = 2 \cdot 10^{-3} \text{ s}^{-1}$.

The schematic diagram of the measuring system is presented in Fig. 3. The specimens were coated with carbon powder to ensure homogeneous emissivity of the specimen. During deformation the film of IR images was obtained (16 frames per second was stored in the hard disk) by means IR camera equipped with system that allows to digitise video signal into numerical one at sampling frequency = 1 MHz. This film was the basis to obtain the temperature distribution on the surface of the strained specimen in course of deformation process. At the same time the stress-strain curves were measured and the straining force as function of deformation time were recorded.

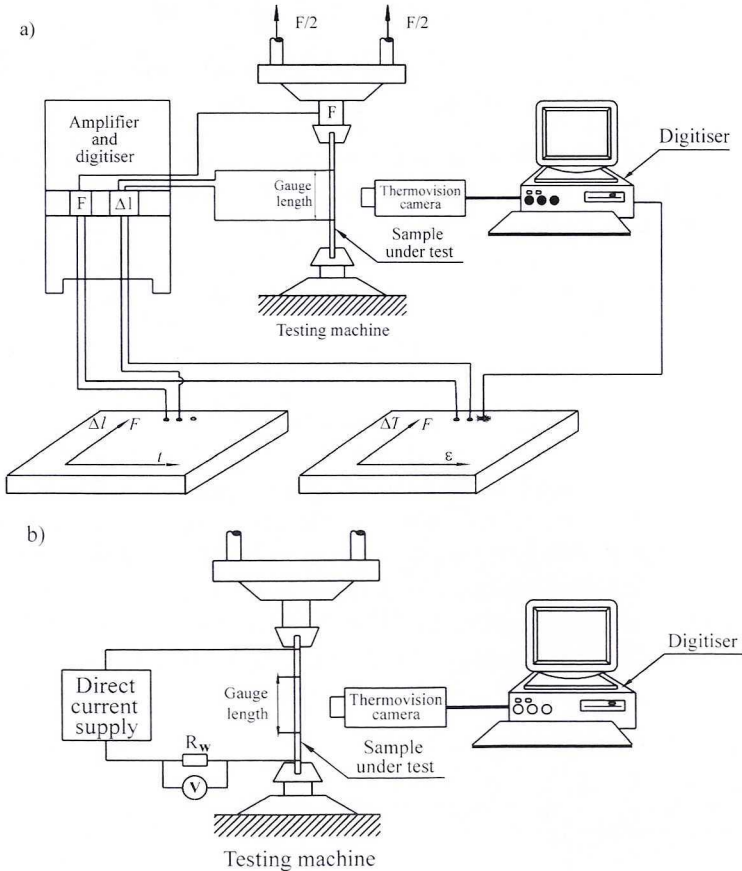


Fig. 3. (a) Schematic diagram of the measuring system designed for the determination of stress-strain curves and the sample temperature during tensile deformation
 (b) Schematic diagram of the measuring system designed for simulation of an increase in the sample temperature

The schematic diagram for simulation of an increase in specimen temperature is shown in Fig. 3b.

During the simulation tests the specimens were mounted in tensile grips in environmental conditions identical with those of the straining experiment. In both cases they were electrically isolated from the machine. The electric power $r(t_1)$ was determined by measuring both the potential difference on the gauge length of the specimen and the current intensity. In order to match the temperature increments during simulation and during tensile testing the electric current and generated power of the heat emission sources must be accurately increase in time. Matching was achieved by employing the method of successive trials. As such a procedure is very laborious, the temperature increases versus time were recorded for various currents and corresponding powers. The family of calibrating $\Delta T(t)$ curves were provided with the electric power as variable parameter. Successive segments of the curve of temperature increase during a tensile test were then matched with corresponding segments of the calibration diagrams. This operation was carried out such that the temperatures corresponding to the starting points of the matching segments were equal to each other. A detailed description of the experimental procedure can be found in Ref. [10].

The method employed for the measurement of the dissipated energy is applicable only within the homogeneous deformation range.

The homogeneity of deformation can be controlled. Isothermal surface of the sample as the indicator of homogeneous deformation in macroscopic scale has been used.

5. Discussion

In polycrystalline metal the slip in individual grains leads to the change of the shape of the grains. This aspect of the slip is seen in relief on the free surface of the deformed specimen as shown in Fig. 4, where grains have random orientation to applied stress.



Fig. 4. Optical micrograph of the specimen surface after strain of 0.045. At this strain de_s/dw_p has the maximum

However, in order to preserve the material continuity within a specimen, additional stresses (accommodation stresses) are generated at the grain boundaries (see introduction).

Fig. 5 shows the dependence de_s/dw_p vs. ϵ^p during tension of fine-grained specimens (curve A, average grain diameter $\approx 8 \mu\text{m}$) and coarse grained specimens (curve B, average grain diameter $\approx 80 \mu\text{m}$). The maximum de_s/dw_p for the fine grained specimens is higher than for coarse grained ones. This may be related to the accommodation stresses generated at the grain boundaries, which are higher in the fine-grained specimens than in the coarse-grained ones. The fine-grained specimens have a greater volume fraction of grain boundaries and consequently more dislocations in the vicinity of the boundaries.

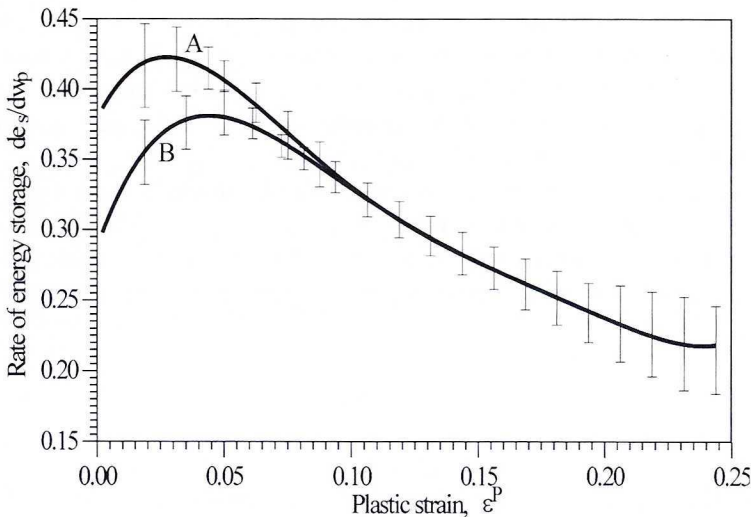


Fig. 5. Dependence of de_s/dw_p on strain obtained during uniaxial tension of austenitic steel for fine-grained (curve A, average grain diameter $\approx 8 \mu\text{m}$) and coarse-grained (curve B, average grain diameter $\approx 80 \mu\text{m}$)

The location of the maximum de_s/dw_p depends on the grain size (Fig. 5). However, after reaching a certain deformation (for the tested steel ≈ 0.10) the plots of de_s/dw_p vs. ϵ^p for the specimens of both groups are practically the same. It means, that after reaching certain strain the grain boundaries have no effect on the processes responsible for the energy storage. Micro-shear banding becomes then the dominating mode of deformation and the grain boundaries have a little effect on the energy storage process.

It has been identified two components of energy storage rate in initial stage of plastic deformation. The first of them is caused by changes in dislocation structures and second one is the result of changes in elastic accommodation stress [13, 14]. A contribution of these components in energy storage process changes with growing strain. In Fig. 5 the resultant rate of energy storage as a function of plastic strain is presented.

On the basis of the experimental results (Fig. 5), and according to equation (14) the attempt have been taken to distinguish the components of the energy storage rate. With the purpose of a partition of the resultant rate of energy storage are made assumptions as follows:

- Contribution of internal stress to the energy storage rate at $\varepsilon^P = 0$ and after reaching a certain deformation (for the tested steel ≈ 0.10) equals zero.
- Decrease of the energy storage rate in dislocation structures is monotonic.

The partition of the resultant rate of energy storage in two components Z_1 and Z_2 is shown in Fig. 6. The variation of the component Z_1 results from change in dislocation structure and the component Z_2 is mainly influenced by generation and decrease of elastic accommodation stress.

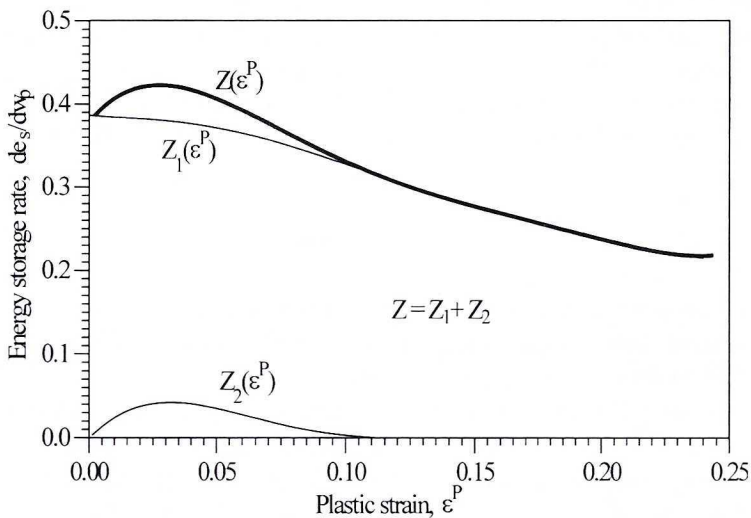


Fig. 6. Decomposition of the rate of storage energy into two components

The component Z_2 appears at the beginning of plastic deformation. It is believed that when this component reaches the maximum value, the change from a homogeneous multi-system slip into micro shear banding in the mode of slip occurs. The decline in Z_2 is the result of the evolution of the micro shear bands that do not generate internal constrains, because of the transgranular nature.

The component Z_1 exists in all tested range of strain. It decreases with growing strain due to the generation of low energy dislocation structure (*LEDSs*).

The preliminary experimental results and results of the theoretical analysis of energy storage rate show what should be done in order determination of the particular of energy stored rate component. Two groups of specimens with primary elongation and one a group without prestrain are required.

The part of steel sheet with homogeneous microstructure should be strained to $\varepsilon \approx 0.07$. On the basis of the presented experimental studies the strain 0.07 corresponds to decline

of the energy storage rate (Fig. 5). From such prepared steel sheet the first group of the specimens should be machined parallel to primary straining direction. The second group should be cut perpendicular to the primary straining. The third group of the samples should be machined from unstrained steel. They will be used as the reference specimens. Then all of samples will be strained in tensile test with a constant strain rate and the energy storage rate as a function of strain will be determined.

It can be expected that during tension of the specimens machined parallel to the primary straining direction non a maximum of the de_s/dw_p occur. During tension of the specimens cut perpendicular to the primary straining the authors expect the maximum of the de_s/dw_p due to first at all a generation of internal stresses. During tension of the specimens without prestrain we will obtain the maximum of the de_s/dw_p resulting as well from the internal stresses as a formation of the dislocation structure. The difference between a functions $de_s/dw_p(\epsilon^p)$ related to the second and the first groups specimens gives the component $Z_2(\epsilon^p)$. The difference between a function $de_s/dw_p(\epsilon^p)$ for specimens without primary straining and $Z_2(\epsilon^p)$ should give the component $Z_1(\epsilon^p)$ due to a rise of dislocation density.

6. Conclusions

It has been shown that the rate of energy storage is a sum of components describing the energy conversion though characteristic internal microscopic mechanisms. This makes possible to identify particular of them.

The analysis of preliminary experimental data arrived at the conclusion that in the initial stage of plastic deformation of polycrystalline metal at least two components of the energy storage rate exist. One of them is associated with the rise of dislocation density, and another one is related to the internal stress field due to elastic accommodation of incompatible strains in the vicinity of grain boundaries.

The experiments have been proposed which enable to distinguish and determinate two components of the energy storage rate in the initial stage of plastic deformation. Thermodynamic description of the experimental method has been presented.

Acknowledgements

Gratitude expressed to the State Committee for Scientific Research (Poland) for financial support under Grant No 7 T08A 046 20.

Paper presentd at the 2nd Symposium "Integrated Study on Basics of Plastic Deformation of Metals", which was held in Łaficut on April 24–27, 2001.

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REVIEWED BY: ANDRZEJ KORBEL

Received: 20 September 2001.