Thermodynamic description of the plastic work partition into stored energy and heat during deformation of polycrystalline materials

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1. Introduction

Inelastic deformation processes of solid bodies are usually characterized by dissipation of part of mechanical energy and storage of some part in the inhomogeneous microstructure. The inelastic (plastic) strains are accompanied by reversible (elastic strains), and during the loading-unloading process, the elastic strain energy is recovered. However, the plastic work w_p expended by mean stress and plastic strain of the representative macro-element is composed of the dissipated part in the form of heat q_d and the residual part e_s stored in the crystalline microstructure. The stored energy is an essential measure of the cold-worked state of the deformed material.

In the description of material under mechanical loading the formalism of irreversible thermodynamics is used. Then the equations of energy and entropy balance (based on the first and the second principles of thermodynamics) expressed in terms of thermodynamic potentials and state variables provide the insight into the energy dissipation and storage. The partition of plastic work into heat and stored energy has been studied in numerous works (Wolfenden, 1968, 1969; Bever et al., 1973; Raniecki and Sawczuk, 1975; Rönnpagel and Schwink, 1978; Oliferuk et al., 1984, 1993, 1995, 1997, 2001, 2004, 2015; Chrysochoos and Maisonneuve, 1985; Chrysochoos et al., 1989, 2009; Chaboche, 1993; Kapor and Nemat–Naser, 1998; Chrysochoos and Louche, 2000; Hodowany et al., 2000; Szczepiński, 2001; Oliferuk and Maj, 2004, 2007, 2009; Rosakis et al., 2004; Ristinmaa et al., 2007; Bodelot et al., 2009; Bartels et al., 2015). In the previous works by Oliferuk et al. it has been shown experimentally that this partition is dependent on the deformation history (Oliferuk et al., 1993, 1995, 2015; Oliferuk and Maj, 2007).

A number of thermo-mechanically coupled plasticity models can be found in the literature (Chaboche, 1993; Kapor and Nemat–Naser, 1998; Ristinmaa et al., 2007; Bartels et al., 2015). The primary objective of those models is to predict the temperature increase of the deformed specimen. But the process of energy storage is a macroscopic manifestation of the changes in the microstructure of the deformed material. This aspect is underlined in the paper by P. Rosakis and his co-workers (Rosakis et al., 2004). The paper is concerned with the fraction,

commonly denoted by β, of the rate of plastic work increment converted into heat to total plastic work increment. The rest of the plastic work increment is converted to the stored energy increment and is related directly to internal variables describing the evolution of the microstructure.

The problem of a plastic deformation description in the framework of thermodynamics which takes into account the internal parameters relating to the microstructure seems to be still open. Therefore, in the presented work we make an attempt to consider parameters characterizing changes in the microstructure of deformed material in a global (average) manner. We do not specify their number nor their structures. The conclusions obtained from the presented considerations will be stated independently of that information. The internal parameters are associated with the macroscopic quantities such as strain and stress entering thermodynamic potentials. Those parameters affect the stored energy because the energy directly depends on changes in the microstructure of the deformed material. Therefore, it is convenient to consider the relationship between the stored energy and the variables characterizing the microstructure. This approach allows us to receive partly integrated form of the Gibbs function comprising the component which presents the stored energy and allows to assess the influence of the configuration entropy on the temperature of deformed specimen. We obtained a relation specifying for the temperature of the deformed specimen. This relation constitutes the theoretical basis for the experimental method of the stored energy determination. The method was used in our previous works (Oliferuk et al., 1984, 1993, 1995, 2001).

A new element with respect to previous works is also the theoretical analysis of the influence of parameters characterizing the changes of microstructure on the thermo-mechanical properties of the deformed material. We have limited ourselves to the analysis of deformation processes that can be considered in macro-scale as homogeneous and quasi-static. Therefore, after a brief presentation of the principles of thermodynamics for the deformed specimen (Section 2), in Section 3 homogeneous processes of plastic deformation have been defined.

In Section 4, the concepts of the thermodynamic reference state and the natural state of the deformed specimen are introduced. The

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difference in the internal energy of the specimen in those states is equal to the stored energy. It is shown that there is no possibility of the stored free energy measurement.

Section 5 deals with the description of the thermodynamic state of the deformed material. An attempt to introduce variables relating to material microstructure into its state description is taken and the incremental equation for temperature is derived.

In Section 6, we look for a thermodynamic basis for a version of energy balance in which the stored energy is an additive component in the expression for the thermodynamic potential.

Section 7 contains the theoretical description of the method of the energy stored determination.

The subject of Section 8 is the energy storage rate and its components related to different modes of deformation. The energy storage rate is the ratio of the stored energy increment to the appropriate increment of plastic work. Experimental results show that the energy storage rate is dependent on plastic strain. This dependence is influenced by different microscopic deformation mechanisms. Here we attempt to refer the components of the energy storage rate to the deformation mechanisms. This is the first step to assign the individual parameters H to those mechanisms.

2. Principles of thermodynamics for the deformed specimen

The first and second principles of thermodynamics for the gauge part of the deformed specimen of mass m and instantaneous volume $V(t)$, can be written in the following form:

$$du = \overline{\overline{d}}w + \overline{\overline{d}}q, \quad \overline{\overline{d}}s^{(p)} \equiv \overline{\overline{d}}s - \overline{\overline{d}}s^{(z)} \geq 0, \tag{2.1}$$

where

$$u = \frac{1}{m} \int_{V(t)} \hat{\rho}\hat{u} \, dV, \tag{2.2}$$

$\hat{\rho}$, $\hat{u}$ are respectively: distributions of the mass density, specific internal energy in micro-scale contained in the volume $V(t)$.

The symbol $\overline{\overline{d}}$ indicates the increment of a quantity which is not an exact differential.

The instantaneous average mass density of the specimen is known as $\rho(t) = \frac{m}{V(t)}$.

An increment of specific mechanical work w expended over the unit mass and an increment of specific heat flux q supplied through the boundary or by heat sources can be expressed as follows:

$$\overline{\overline{d}}w = \frac{dt}{m} \int_{\partial V(t)} \hat{\mathbf{t}}^{(n)} \cdot \hat{\mathbf{v}} da, \quad \overline{\overline{d}}q = \frac{dt}{m}\left[-\int_{\partial V(t)} \hat{\mathbf{q}} \cdot \mathbf{n} \, da + \int_{V(t)} \hat{\rho}\hat{r} dV \right], \tag{2.3}$$

where $\hat{t}$ and $\hat{q}$ are: the vector of the traction distribution and the distribution of the heat flux on the specimen boundary surface $\partial V(t)$, v is velocity of micro-particles contained in the volume $V(t)$ in the time interval from t to $t + \Delta t$, $\hat{r}$ denotes the rate of heat sources and $\mathbf{n}$ is the unit vector normal to the surface $\partial V(t)$.

Micro-scale phenomena taking place during plastic deformation can cause an increase in entropy of deformed specimen. Denote the increment of the specific entropy produced due to microstructure evolution as $\overline{\overline{d}}s^{(p)}$. Then

$$\overline{\overline{d}}s^{(p)} = ds - \overline{\overline{d}}s^{(z)} \geq 0,$$

where ds is the increment of average specific entropy of the tested specimen and $\overline{\overline{d}}s^{(z)}$ is the increment of averaged specific entropy due to heat flow from the exterior and due to heat sources $\hat{r}$. Here:

$$ds = \frac{1}{m} \int_{V(t)} \hat{\rho}\hat{s} dV, \quad \overline{\overline{d}}s^{(z)} = \frac{dt}{m}\left[-\int_{\partial V(t)} \frac{\hat{\mathbf{q}} \cdot \mathbf{n}}{\hat{T}} \, da + \int_{V(t)} \frac{\hat{\rho}\hat{r}}{\hat{T}} dV \right], \tag{2.4}$$

where $\hat{s}$ i $\hat{T}$ are the fields of specific entropy and temperature in the micro-scale.

3. Homogeneous processes of plastic deformation

We confine ourselves to the analysis of processes that can be considered as the homogeneous. These processes must satisfy the following conditions:

a) the average velocity of specimen micro-particles is zero,
b) the temperature field is uniform,

$$\hat{T} = T(t). \tag{3.1}$$

c) the surface traction on the specimen surface $\partial V(t)$ is uniform and has the following form:
For the homogeneous process of plastic deformation

$$\overline{\sigma}_{ij}(t) = \sigma_{ij}(t). \tag{3.4}$$

If the macroscopic stress σ_{ij} induced by loading vanishes, then in the tested specimen exists only a balanced (or residual) stress field induced by the lattice defects and related to the internal strain distortion.

d) If during the experiment the displacement velocity is controlled on the element boundary $\partial V(t)$ then the distribution of the velocity field is limited to the following form:

$$\hat{t}_i = \sigma_{ij}(t)n_j, \tag{3.2}$$

where the components of the stress tensor σ_{ij} do not depend on the position of particles on the surface of the specimen $\partial V(t)$. The average stress in the gauge part of the specimen is defined as follows:

$$\overline{\sigma} \equiv \frac{1}{2V(t)} \int_{\partial V(t)} (\hat{\mathbf{t}}^{(n)} \otimes \mathbf{x} + \mathbf{x} \otimes \hat{\mathbf{t}}^{(n)}) \, da = \frac{1}{V(t)} \int_{V(t)} \hat{\sigma}(x, t) dV. \tag{3.3}$$

where $\mathbf{x}$ is the vector-radius and denotes the dyadic product, $t \otimes \mathbf{x} = t_i x_j$.

$$\hat{v}_i = D_{ij}(t)x_j + \Omega_{ji}(t)x_j, \quad x \in \partial V(t) \tag{3.5}$$

where $D_{ij}(t) = D_{ji}(t)$ denotes a macroscopic Euler strain rate, $\Omega_{ij}(t) = \Omega_{ji}(t)$ is a rigid rotation rate measure of the gauge part of the specimen.

The average strain is defined as follows:

$$\overline{\mathbf{D}} = \frac{1}{2V(t)} \int_{\partial V(t)} (\hat{\mathbf{v}} \otimes \mathbf{n} + \mathbf{n} \otimes \hat{\mathbf{v}}) \, da = \frac{1}{V(t)} \int_{V(t)} \hat{\mathbf{D}}(x, t) dV. \tag{3.6}$$

Here $\overline{\mathbf{D}}$ represents the average value of the micro-strain rate field $\hat{D}(x,t)$, assuming the micro-strains to be generated by the kinematically admissible velocity field satisfying Eq. (3.5),

$$\overline{D}_{ij} = \hat{D}_{ij}(t). \tag{3.7}$$

Then the increment of mechanical work w expended over the unit mass has the following form:

$$\overline{\overline{d}}w = \frac{\overline{\sigma}_{ij}(t)\overline{D}_{ij}(t)}{\rho(t)} dt, \tag{3.8}$$

$\overline{\overline{d}}w$ is expressed by the product of the average values of the stress field and of the strain rate field divided by the mass density $\rho(t)$.

Substituting (3.1) into (2.4)$_2$, with account for (2.3)$_2$ and assuming that the average velocity of specimen micro-particles is zero, we obtain $\overline{\overline{d}}s^{(z)} = \frac{\overline{\overline{d}}q}{T}$. Therefore the first and the second principles of thermodynamics for infinitesimal, quasi-static, homogeneous processes can be written as:

$$du = \overline{\overline{d}}w + \overline{\overline{d}}q, \quad T\overline{\overline{d}}s^{(p)} \equiv \overline{\overline{d}}w_D = Tds - \overline{\overline{d}}q \geq 0, \tag{3.9}$$

where $\overline{\overline{d}}w$ is defined by (3.8) and $\overline{\overline{d}}w_D$ is the increment of the dissipated