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# The stored energy of plastic deformation in crystals of face-centered cubic metals

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**Abstract.** This article presents the results of investigation into changes in the stored energy during the process of plastic deformation. It has been shown that the value of stored energy increases with the degree of deformation and the higher this value the lower the deformation temperature. The stored energy decreases with increasing temperature. Intervals of strong and weak temperature dependence are associated with changes in the intensity of accumulation of deformation defects of different types. The stored energy also increases with increasing stress and the degree of deformation, which corresponds to the experimental data.

## 1. Introduction

Metals and alloys are in a state far from thermodynamic equilibrium in the process of plastic deformation. Excess energy that is stored in plastic deformation is an important integral characteristic of the defect structure of deformed material [1-3]. During the process of deformation and after its finish, relaxation processes occur in the deformed material: the restructuring in deformation defect structure in the direction of reducing the stored energy. After the termination of the deforming impact absorbed energy is the driving force behind relaxations' changes of the structure.

A lot of experimental data on the energy absorption in metals during plastic deformation and release of this energy during annealing post-deformation were obtained [1-3, 4].

In publication [4] were presented results of study on the thermo-mechanical responses and properties of single crystal high purity copper. The authors obtained that the stored energy of cold work depends almost linearly on the plastic strain for all different strain rates from 1000 to 8000 s<sup>-1</sup>, and therefore the stored energy is on relative independence on the strain rate.

In theoretical study [5] was demonstrated that the significant part of the energy stored during deformation of tested materials is the energy of statistically stored dislocations and their mutual interactions. A method for the calculation of the stored energy was presented in publication [6]. The authors indicate that the stored energy increases with increasing hardening capacity of the metal.

Only a small part of the energy consumed by plastic deformation of the metal is absorbed by the crystal, thereby increasing its internal energy. The increase of internal energy is connected to defects arising during deformation; and it generates a driving force of recovery and recrystallization. The contribution to the change in the stored energy can produce various defects, including dislocations, point defects, microcracks, etc. Value of stored energy depends upon different factors associated with the process of deformation, and with the nature of the deformation material undergoing deformation.



The aim of the present work is to research of the stored energy of plastic deformation in crystals of face-centered cubic metals over a wide range of temperatures.

## 2. Mathematical model

In previous studies [7-9] the stored energy for isothermal and adiabatic deformation at a constant strain rate, annealing of the stored energy of deformation during isothermal annealing and annealing with a constant heating rate of material were calculated on based model [10]. The model [10] takes into account generating of deformation of point defects at a stationary density of thresholds in dislocations and without account the generation of dislocation dipoles.

The model [10] qualitatively correctly describes the general patterns of energy-absorbing deformation and its release during annealing. We have also shown that the value of the stored energy, taking into account the dynamic generation of point defects and dislocation dipoles leads to a better agreement with the experimental data.

In the present study the stored energy is defined by  $E = E_s d\rho + E_{id}$ , where  $E$  is the stored energy per unit length of the dislocation,  $E_s$  is the self-energy per unit length of dislocation [11]:

$$E_s = \frac{Gb^2}{4\pi K} \cdot \ln \frac{R}{r}, \quad (1)$$

where  $G$  is the shear modulus,  $b$  is Burgers vector module,  $R$  is the characteristic size of the region outside of which the energy of elastic distortions caused by the presence of dislocations is negligible;  $K = 1$  for screw dislocations,  $K = 1 - \nu$  for screwless dislocation respectively,  $E_{id}$  is the energy of the interaction of dislocations, and  $r$  is the radius of the dislocation core.

According to the publication [12] the self-energy per unit length of the dislocation can be calculated taking into account the energy of the dislocation core as follows:

$$E_s = \frac{Gb^2}{4\pi K} \cdot \ln \frac{R}{r} + E_c \quad (2)$$

The energy of the dislocation core  $E_c$  was estimated in the study [13] and it can be written as:

$$E_c = 0.1 E_s. \quad (3)$$

It is used in calculations that  $r = 2b$ ,  $R = 6\rho^{-1/2}$ . The relations (1)-(3) show that the energy of the dislocation core is small compared with the first term included in (2), as a consequence the energy of the dislocation core is often neglected. In further calculations for the contribution to the stored energy due to the accumulation of dislocations with the energy of the dislocation core will use the relation:

$$\Delta E_m = 1.1 \frac{Gb^2}{4\pi} K^{-1}(\psi)(\rho_m - \rho_m^0) \ln \frac{R}{r}, \quad (4)$$

where  $K(\psi) = \frac{1}{2}(2-\nu)/(1-\nu)$ ,  $\rho_m^0$  – the initial density of shear-forming dislocations. The energy of the dislocations in the dipole configurations is represented in the form

$$\Delta E_d = \frac{Gb^2}{4\pi(1-\nu)} \rho_d \ln \frac{\langle h \rangle}{r}, \quad \text{and } \langle h \rangle = \frac{G(2-\nu)}{8\pi\tau_f(1-\nu)} b, \quad (5)$$

where  $\langle h \rangle$  is a average dipole arm, which is used to work in a uniform distribution of dipoles along the length of the arm.

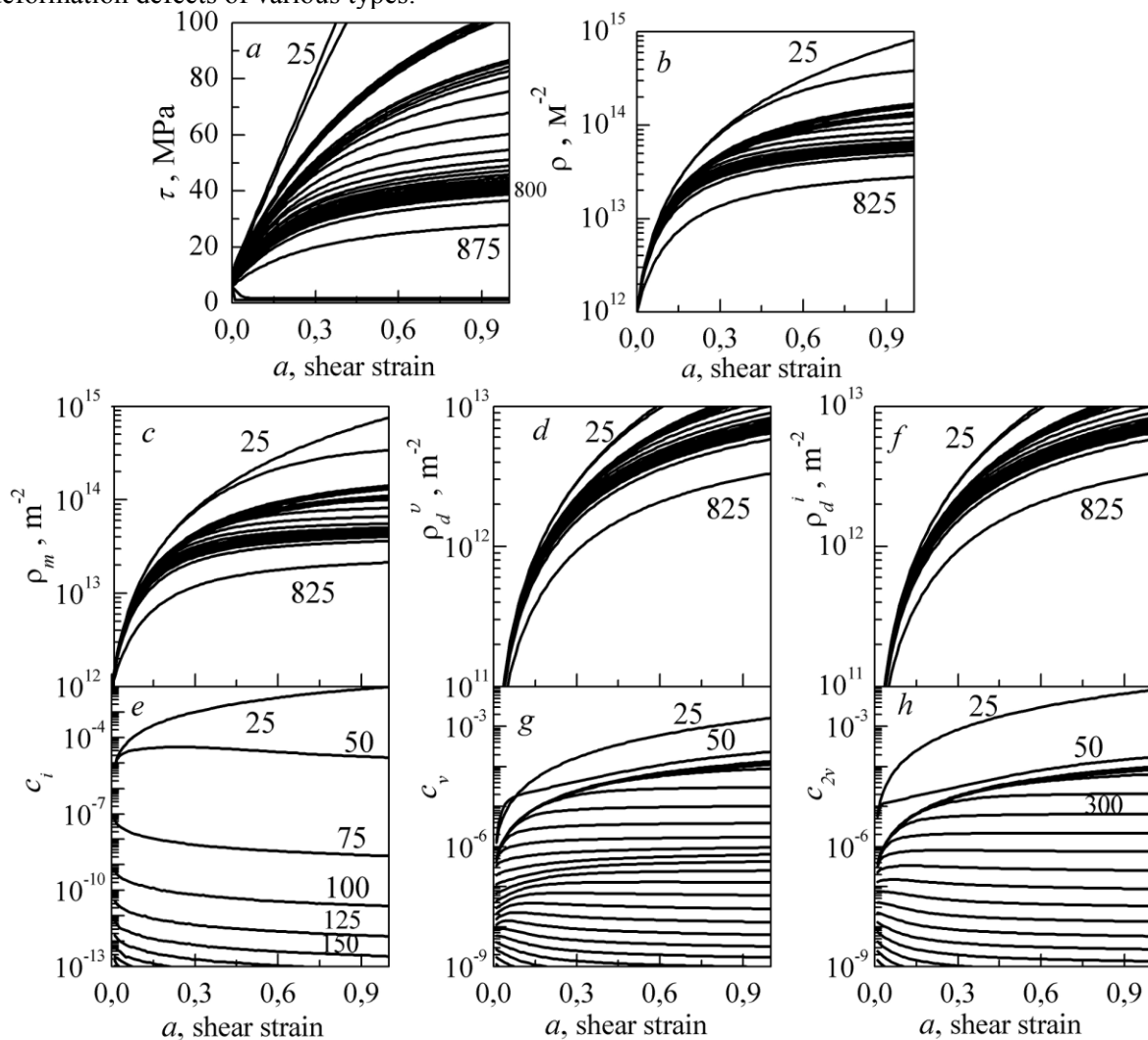
The main source of strain hardening of metals is the accumulation of dislocations during plastic deformation, so the existing theoretical works [14] devoted to the stored energy usually considered only the contribution due to the accumulation of dislocations, the contribution of point defects are usually not taken into account. In this paper, the calculation takes into account the contribution of the stored energy of point defects, which is also associated with increase in stored energy. If the concentration of defects exceeds the thermodynamic equilibrium, the stored energy of the crystal is increased by an amount equal to the number of defects multiplied by the energy of formation of a single defect, assuming the formation of isolated point defects assuming the formation of isolated

point defects:

$$\Delta E_v = n_v U_v^f \approx \frac{c_{1v}}{b^3} U_v^f, \quad \Delta E_{2v} = n_{2v} U_{2v}^f \approx \frac{c_{2v}}{2b^3} U_{2v}^f, \quad \Delta E_i = n_i U_i^f \approx \frac{c_i}{2b^3} U_i^f, \quad (6)$$

here  $n_v$ ,  $n_{2v}$ ,  $n_i$  – the number of vacancies, divacancies and interstitial atoms per unit volume, respectively;  $c_v$ ,  $U_v^f$ ,  $c_{2v}$ ,  $U_{2v}^f$ ,  $c_i$ ,  $U_i^f$  – concentration of point defects and their formation energy, respectively. Then using relations (4)-(6) for the absorbed energy of deformable material assuming an additive contribution can be written  $\Delta E = \Delta E_m + \Delta E_d + \Delta E_p + \Delta E_v + \Delta E_{2v} + \Delta E_i$ .

Dependences of the stored energy from the flow stress and shear strain  $\rho(\tau)$ ,  $\rho(a)$ ,  $c_{1v}(\tau)$ ,  $c_{2v}(\tau)$ ,  $c_i(\tau)$  can be determined by solving the system of equations of mathematical model of homogeneous plastic deformation in FCC materials [14]. The mathematical model [14] together with the relations (4)-(6) allows us to calculate the absorbed energy of deformable material and contributions to it energy of deformation defects of various types.



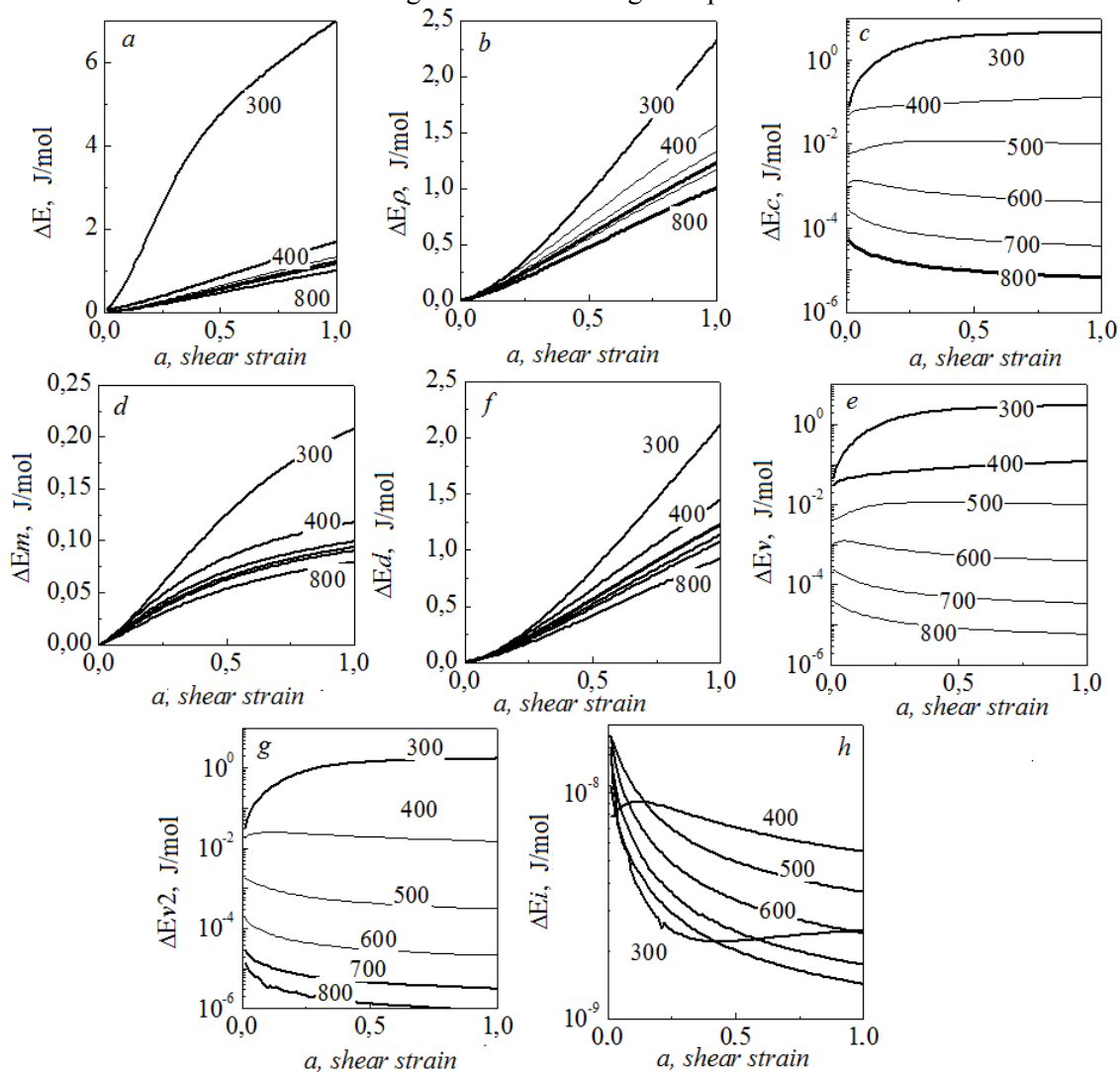
**Figure 1.** Flow stress (a), density of shear-forming dislocations (b), density in the dipole configuration (b), (c), concentration of interstitial atoms (e), vacancies (g), and divacancies (h) versus strain rate. Copper, temperature from 25 to 900 K in steps of 25 K.

### 3. Results of numerical experiments

Stress-strain curves and the corresponding dependence of the density of dislocations, shear-forming dislocations, dislocations in dipole configurations of vacancy and interstitial type and concentration of

interstitial atoms, vacancies, divacancies versus strain for copper are shown in Figure 1, for deformation temperatures from  $T=25$  K to 900 K in step of 25 K. As the temperature decreases the strain hardening coefficient and steady-state value of the flow stress are reduced (Figure 1, *a*). The temperature intervals of strong and weak temperature dependence associated with changes in the intensity of the annihilation of deformation defects of different types were found. It should be noted that unlike the model-shear deformation diffusion, in which the density of dislocation dipole is greater than the density of shear-forming dislocations, in presented model [14] the density of shear-forming dislocations is higher than the density of the dislocation dipole or comparable with it.

For each type of dislocation range of temperature dependence can be identified corresponding to the intervals of the temperature dependence of strain hardening. At temperatures above  $T=100$  K the concentration of interstitial atoms in deformed crystal is negligible, less than  $c_i=10^{-9}$ . The concentration of vacancies even during deformation at high temperatures of at least  $c_v=10^{-9}$ .



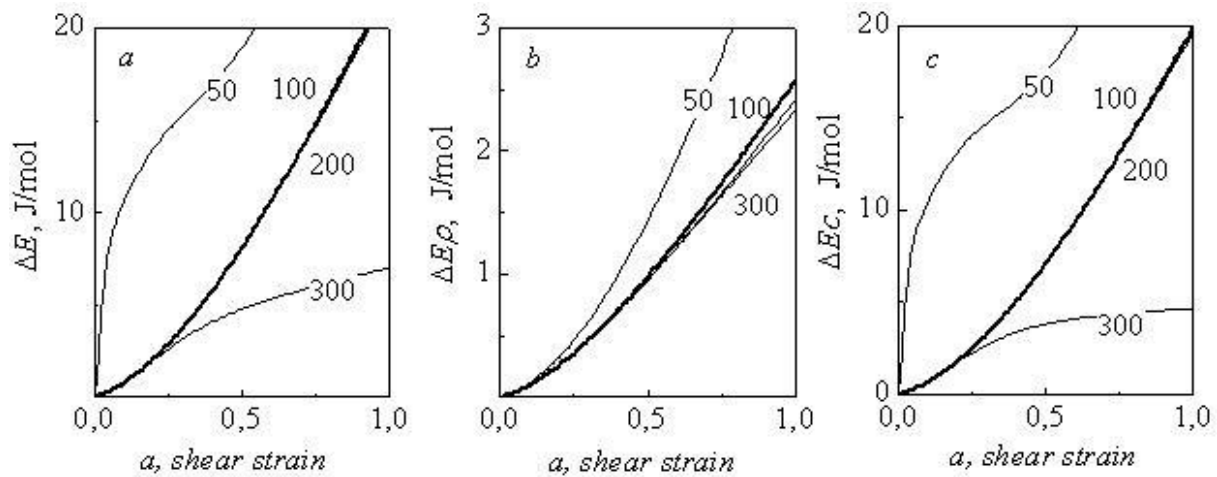
**Figure 2.** Stored energy (a) and contributions to it dislocations (b), point defects (c) shear-forming dislocations (d), dislocations in the dipole configuration (e), vacancies (f), divacancies (g), and interstitial atoms (h) versus the shear strain for copper. Temperature varied from  $T=300$  to 800 K in steps of 100 K.

Figures 2-4 show the results of our calculations of stored energy based on the developed model [14]. It has been shown that the quantity of stored energy increases with the degree of deformation and the more intense the lower the deformation temperature. With increasing temperature, the stored strain

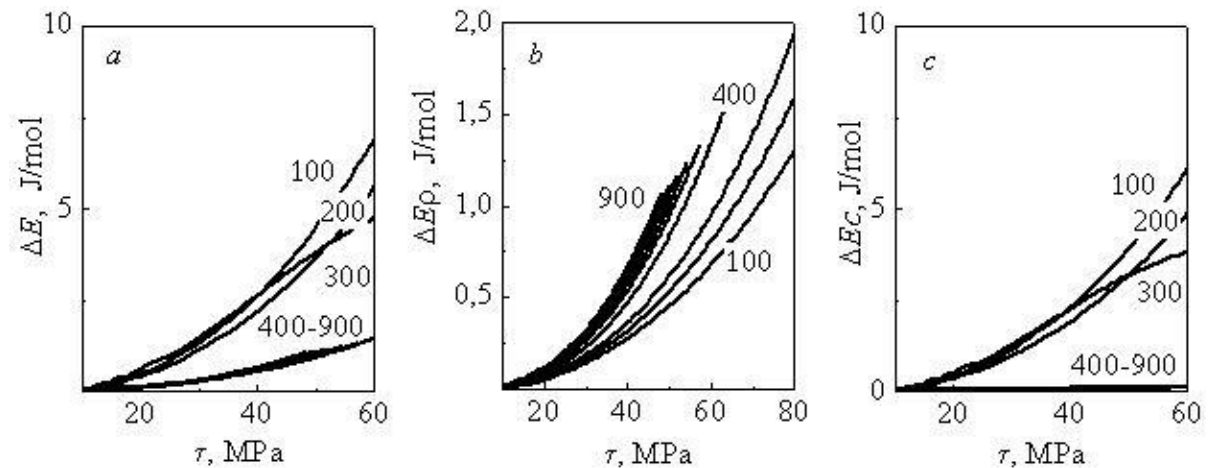
energy is reduced (Figure 2).

It was found that the temperature intervals of strong and weak temperature dependence is associated with changes in the intensity of accumulation of deformation defects of different types. The contribution of point defects in the stored energy at low temperatures may exceed the contribution of dislocations or be commensurated with it. The contribution of point defects in the stored energy is determined by the contribution of di- and vacancy, contribution of interstitial atoms is negligible. But starting with the temperature of about  $T=400$  K for copper the contribution of point defects by orders of magnitude is smaller than that of dislocations.

Figure 3 shows the curves of the stored energy at low temperatures (up to  $T=300$  K in steps of 50 K). By increasing the temperature to room temperature the contribution into the stored energy of point defects is significantly reduced, while the contribution from the dislocation remains virtually unchanged. Stored energy increases with increasing tension (Figure 4) and the degree of deformation, which corresponds to the experimental data.



**Figure 3.** Stored energy (a) and deposits it dislocations (b), and point defects (c) versus the shear strain for copper. Temperature varied from  $T=50$  to 300 K in steps of 100 K.



**Figure 4.** Stored energy (a) and contributions to it dislocations (b), point defects (c) versus the flow stress for copper.

#### 4. Conclusion

The absolute values of the stored energy correspond to the order of data in the literature [1, 3, 11, 14, 15, 16]. The following basic laws of energy absorption of single crystals of fcc metals are noted, in agreement with the experimental data: 1) the amount of stored energy increases with the degree of deformation and the more intense the lower the temperature; 2) the quantity of stored energy higher at higher deformation strain rate, at low temperatures increasing strain rate has a little effect on the accumulation of energy. From the numerical experiments embodied in Figures 1-4 it may be concluded that the proposed mathematical model can be used in the prediction of plastic deformation processes under different external impacts.

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