

## THE INFLUENCE OF TEMPERATURE AND STRAIN RATE ON THE STRENGTHENING OF METALLIC MATERIALS

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### Abstract

Extensive literature indicates that the effect of strengthening materials is related to their structural construction. The structure of the metallic material exhibits the greatest strengthening effect when there is a very limited movement of dislocations and their movement is completely blocked due to numerous obstacles [1, 3, 6-9, 12, 15, 16].

In this paper strain, rate and temperature dependences of yield strength of metallic materials are presented. The effect of temperature and strain rate on the value mechanical threshold stress is determined.

In addition, the effect of temperature on the Kirchhoff modulus and Burgers vector is determined. The interaction of dislocations with grain boundaries causes additional stress – athermal stress causing the strengthening of the structure. The term “athermal” implies that thermal activation is unable to assist the dislocation past these obstacles.

The strengthening of metallic materials is related to the dimensions of the grains, which influence the athermic stress.

The calculations of mechanical threshold stress and other parameters of the structure of the material allow for easier understanding of the strengthening of the material loaded with temperature and strain rate. The largest strengthening occurs in pure metals and their alloys in the case of the total blocking of dislocation motion. This process takes place when the temperature is 0 K or at very high strain rates.

The metal demonstrates the greatest effort, which is called mechanical threshold stress (MTS) [5].

**Keywords:** strengthening materials, dislocations, athermic stress, mechanical threshold stress (MTS)

### 1. The influence of temperature and strain rate on the selected properties of metallic materials according to dislocation theory

The dependence describing mechanical threshold stress  $\hat{\sigma}$  is the constitutive model, which relates to internal state changes  $\hat{\sigma}$  depending on the temperature and strain rate [5]

$$\sigma = \left[ 1 - \frac{kT}{G} \ln \left( \frac{\dot{\epsilon}_0}{\dot{\epsilon}} \right) \right] \hat{\sigma}. \quad (1)$$

The equation (1) is a dependence of the plasticizing stress (yield strength) from the temperature, strain rate and MTS  $\hat{\sigma}$ . State variables of the above model can be written as

$$\sigma = s(\dot{\epsilon}, T, ) \hat{\sigma}, \quad (2)$$

where:

$$s(\dot{\epsilon}, T) = \left[ 1 - \frac{kT}{G} \ln \left( \frac{\dot{\epsilon}_0}{\dot{\epsilon}} \right) \right]. \quad (3)$$

Figure 1 shows two stacked planes that correspond to the hexagonal close-packed (HCP) as the densest packing of hexagonal structure and the face-centered cubic (FCC). Such a close-packed structure does not correspond to the body-centered cubic (BCC).

It is only possible to apply a force to each row of atoms on the top plane and slide them over the bottom plane. Such method of generating “permanent” strain would create a movement of

material in the top plane in relation to the bottom plane [5]. Fig. 2 presents the side view of planes position; there is an impression of a single row movement, instead of whole plane.

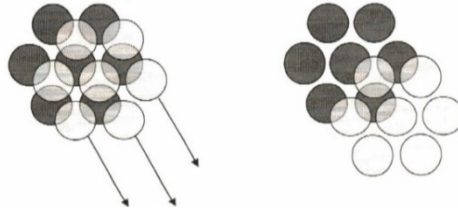


Fig. 1. Two close-packed planes with one sliding over the other [5]

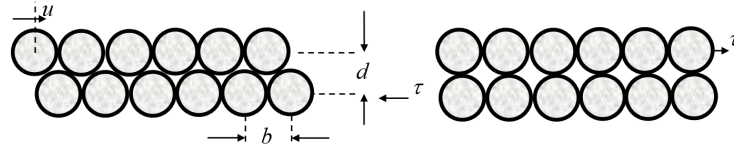


Fig. 2. A side view of the configuration shown in Fig. 1 [5]

On the basis of Fig. 2, the shear stress  $\tau$  will be 0 when  $u = 0$  (equilibrium position) and when  $u = b/2$  (right-hand side). The stress to impose the elastic motion is related to the strain through [5]:

$$\tau = \mu\lambda = \mu \frac{u}{d}, \quad (4)$$

where:

$\mu$  – shear modulus,

$\lambda$  – shear strain.

This equation (4) allows motion of the top plane relative to the bottom plane description. According to dislocation theory, the stress in the metallic material structure is a result of the interaction of a dislocation with a variety of obstacles. In all cases, the stress value is proportional to the shear modulus. Dislocation theory predicts that the stress to bend a dislocation to a radius  $R_d$  is [5, 10]:

$$\tau \approx \frac{\mu \cdot b}{2 \cdot R_d}, \quad (5)$$

where:

$\mu$  – shear modulus,

$b$  – burgers vector,

$R_d$  – radius of a dislocation loop [10].

In reality, there is no clear screw dislocation or edge dislocation, but meets dislocation loops. Part of the loop is a screw, and a part of the edge, but the greater part is mixed edge and screw. Studies have shown that the yield strength, shear modulus and Burgers vector are function of temperature. However, values Burgers vector and of the shear modulus values depend on temperature in small extent while the yield stress is strongly dependent on the temperature. To take into account such dependencies the Equation (1) can be rewritten as:

$$\frac{\sigma}{\mu} = \left[ 1 - \frac{kT}{G} \ln \left( \frac{\dot{\epsilon}_0}{\dot{\epsilon}} \right) \right] \frac{\hat{\sigma}}{\mu_0}, \quad (6)$$

where:  $\mu$  – shear modulus at  $T$  temperature,  $\mu_0$  – shear modulus 0 K temperature:

$$\mu_0 = \mu|_{T=0K}. \quad (7)$$

In polycrystals, the strength addition due to interaction of dislocation with grain boundaries, it is expressed in the form athermal stress,  $\sigma_a$ . The term “athermal” implies that thermal activation is unable to assist the dislocation past these obstacles.

This is evidenced by the martensite transformation in iron alloys: austenite (FCC – face – centered cubic structure) → supersaturated with carbon the ferrite (BCC – body centered cubic structure). The driving force of the transformation is the difference of free energies of austenite and martensite.

The dependence between the yield point and stress along the slip plane of the grain boundaries, the grain size and the athermal stress is described by Hall – Petch equation [5]:

$$\sigma = \sigma_i + \frac{k_d}{\sqrt{d_{gs}}}, \quad (8)$$

where:

$d_{gs}$  – grain dimension,

expression  $k_d \cdot d_{gs}^{-1/2}$  – the grain size and is called the athermal stress  $\sigma_a$ ,

$k_d$  – proportionality constant in the Hall-Petch equation,

$\sigma_i$  – stress (e.g. related to  $\tau_{CRSS}$  – critical resolved shear stress in a pure metal) in a material with a very low dislocation density.

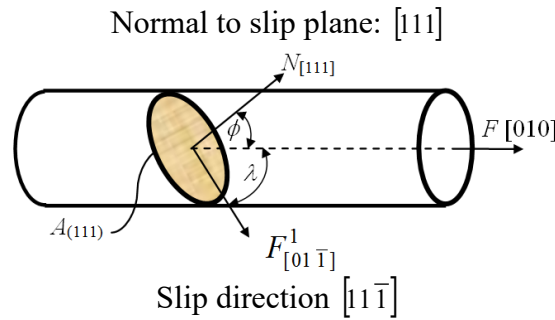


Fig. 3. Slip planes and directions for a single crystal with a slip plane at an angle  $\phi$  and a slip direction at an angle  $\lambda$  to the stress axis [5]

Figure 3 shows a scheme stretching the specimen. Two angles have been defined, a first ( $\phi$ ) between the load axle ( $F$ ) and perpendicular to the slip plane ( $N$ ) and a second ( $\lambda$ ) between the load direction ( $F$ ) and load constituent to the sliding direction ( $F^l$ ).

A slide starts sequentially under the planes and the directions in which the tangential component of the stress at the earliest reaches a critical size ( $\tau_{CRSS}$ ). The value of the tangential stress caused by the external load depends on the slip plane and direction. Stress cutting at the slip is the quotient of a force in the slip direction by the skid surface:

$$\tau = \frac{F_{[01\bar{1}]}}{A_{(111)}}. \quad (9)$$

The stress  $\tau$  is called the critical resolved shear stress  $\tau_{CRSS}$ . With regard to the sample surface  $A$ :

$$A_{(111)} = \frac{A}{\cos \phi}. \quad (10)$$

The value of the force in the slip direction:

$$F_{[01\bar{1}]} = F \cos \lambda. \quad (11)$$

Hence:

$$\tau_{CRSS} = \frac{F_{[01\bar{1}]}}{A_{(111)}} = \frac{F \cos \lambda}{\frac{A}{\cos \varphi}} = \frac{F}{A} \cos \varphi \cos \lambda = \sigma_{cr} \cos \varphi \cos \lambda. \quad (12)$$

Factor  $[\cos \varphi \cos \lambda]$  is defined as a Schmidt factor, its value is less or equal to unity and the stress  $\sigma$  is tensile stress [4]. The critical resolved tensile stress  $\sigma_{cr}$  is equivalent of the yield strength at tensile [2].

Equation (1) after taking into account stress  $\sigma_a$  is presented below:

$$\sigma = \sigma_a + s(\dot{\varepsilon}, T) \hat{\sigma}. \quad (13)$$

Athermic stress  $\sigma_a$  is equivalent to the expression:  $k_d / \sqrt{d_{gs}}$ . Equation (6) after taking into account athermal stress:

$$\frac{\sigma}{\mu} = \frac{\sigma_a}{\mu} + \left[ 1 - \frac{kT}{G} \ln \left( \frac{\dot{\varepsilon}_0}{\dot{\varepsilon}} \right) \right] \frac{\hat{\sigma}}{\mu_0}. \quad (14)$$

Between the activation energy  $G$  and the shear modulus, there is a simple relationship:  $G = \mu \cdot b^3$ . Equation (14) including the mentioned dependency is presented below:

$$\frac{\sigma}{\mu} = \frac{\sigma_a}{\mu} + \left[ 1 - \frac{kT}{g_0 \mu b^3} \ln \left( \frac{\dot{\varepsilon}_0}{\dot{\varepsilon}} \right) \right] \frac{\hat{\sigma}}{\mu_0}. \quad (15)$$

where  $g_0$  – normalized activation energy.

The benefit of this normalization is that  $g_0$  values become dimensionless and closer to unity [5]. After transforming the equation (15) the following dependency can be obtain:

$$\frac{\sigma - \sigma_a}{\mu} = \left[ 1 - \frac{kT}{g_0 \mu b^3} \ln \left( \frac{\dot{\varepsilon}_0}{\dot{\varepsilon}} \right) \right] \frac{\hat{\sigma}}{\mu_0}. \quad (16)$$

## 2. Determination of the mechanical threshold stress and the yield stress

Samples of molybdenum have been tensiled with different strain rate and at different temperatures. For each strain rate and for each temperature the stress values were determined. On the basis of the work (Table E6.3 [5]) were presented research results in Tab. 1. Burgers vector length for molybdenum is 0.26 nm. The shear modulus is a function of the temperature, the athermic stress is equal  $\sigma_a = 100$  MPa while  $\dot{\varepsilon}_0 = 10^8 \text{ s}^{-1}$ .

The objective is to determine the value of the mechanical threshold stress  $\hat{\sigma}$  and the factor of normalized activation energy  $g_0$ .

To determine the value  $\hat{\sigma}$  and  $g_0$  the equation (15) was used. Data are  $\sigma_a = 100$  MPa,  $\dot{\varepsilon}_0 = 10^8 \text{ s}^{-1}$ ,  $b = 0,26$  nm,  $k = 1.38 \cdot 10^{-23} \text{ J/K}$  and on the basis of Tab. 1  $T$ ,  $\dot{\varepsilon}$ ,  $R_e$ . Shear modulus  $\mu(T)$  on a function of temperature was determined on the basis to the Varshi equation [5, 18]:

$$\mu(T) = \mu_0 - \frac{D_0}{\exp\left(\frac{T_0}{T}\right) - 1}. \quad (17)$$

Tab. 1. Results of measuring the yield strength of molybdenum depending on temperature and strain rate [5]

Temperature, K	Strain rate, s <sup>-1</sup>	Yield strength, MPa
200	0.001	1124
300	0.001	998
400	0.001	897
500	0.001	799
200	1.0	1156
300	1.0	1090
400	1.0	1002
500	1.0	934
200	2000	1203
300	2000	1167
400	2000	1125
500	2000	1065

For molybdenum, it was assumed (on the literature basis) [5]:

$$\mu_0 = 142.7 \text{ GPa}, D_0 = 6.475 \text{ GPa}, T_0 = 252 \text{ K}.$$

Based on data presented in the Tab. 1:

$T_1 = 200 \text{ K}, T_2 = 300 \text{ K}, T_3 = 400 \text{ K}, T_4 = 500 \text{ K}, \dot{\epsilon}_1 = 10^{-3} \text{ s}^{-1}, \dot{\epsilon}_2 = 1,0 \text{ s}^{-1}, \dot{\epsilon}_3 = 2 \cdot 10 \text{ s}^{-1}$ , shear modulus values were determined using the dependence (17):

$$\mu(\cong 0) = 142.7 \text{ GPa}, \mu(200) = 140.1 \text{ GPa}, \mu(300) = 137.8 \text{ GPa}, \mu(400) = 135.3 \text{ GPa}, \mu(500) = 132.8 \text{ GPa}.$$

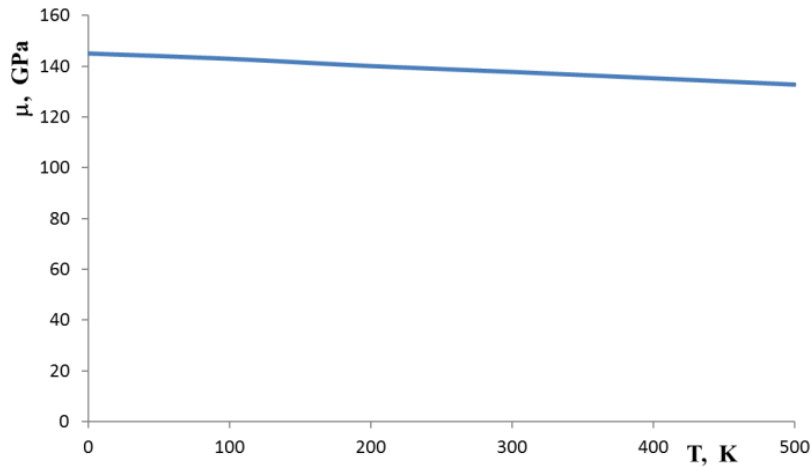


Fig. 4. The change the shear modulus value as a function of temperature for the molybdenum

Figure 4 shows the change of the shear modulus value depending the temperature for the molybdenum. Change of the shear modulus  $\mu$  value dependent on the temperature for the molybdenum (Fig. 4) is small.

The mechanical threshold stress of molybdenum has been defined by the transformation of the equation (16):

$$\hat{\sigma} = \frac{\sigma \cdot \mu_0}{\sigma_a \cdot \left[ 1 - \frac{kT}{g_0 \mu b^3} \ln \left( \frac{\dot{\epsilon}_0}{\dot{\epsilon}} \right) \right]},$$

for the calculations, it was assumed:

$$\sigma_1 = 1124 \text{ MPa}, T_1 = 200 \text{ K}, \dot{\varepsilon}_1 = 10^{-3} \text{ s}^{-1}, b = 0.26 \text{ nm}, \mu_0 = 142.7 \text{ GPa}, \dot{\varepsilon}_0 = 10^8 \text{ s}^{-1},$$

1)

$$\sigma_a = 100 \text{ MPa}, k = 1.38 \cdot 10^{-23} \text{ J/K}, \mu_1(200) = 140.1 \text{ GPa},$$

hence:

$$\text{a) } \hat{\sigma} = \frac{1.6 \cdot 10^{12} \cdot g_0}{g_0 - 0.0285},$$

$$\sigma_2 = 799 \text{ MPa}, T_2 = 500 \text{ K}, \dot{\varepsilon}_2 = 10^{-3} \text{ s}^{-1}, b = 0.26 \text{ nm}, \mu_0 = 142.7 \text{ GPa}, \dot{\varepsilon}_0 = 10^8 \text{ s}^{-1},$$

2)

$$\sigma_a = 100 \text{ MPa}, k = 1.38 \cdot 10^{-23} \text{ J/K}, \mu_2(500) = 132.8 \text{ GPa},$$

$$\text{b) } \hat{\sigma} = \frac{1.14 \cdot 10^{12} g_0}{g_0 - 0.075}.$$

When comparing dependence a) and b) the following results were obtained:

$$g_0 = 0.2 \text{ and } \hat{\sigma} = 1860 \text{ GPa}.$$

The equation (1) as a general form for equation (15) that is describing the variation of yield stress depending on its temperature and strain rate.

It should be noted that this expression represents the shape of the obstacle profile and the form of the equation (15) represents a highly idealized profile. A further modification to equation (1) is to introduce parameters that more accurately represent “curvature” of the obstacle profile through the exponents  $p$  and  $q$  put into equation (18) [5, 11]:

$$\left( \frac{\sigma - \sigma_a}{\mu} \right)^p = \left\{ 1 - \left[ \frac{kT}{g_0 \mu b^3} \ln \left( \frac{\dot{\varepsilon}_0}{\dot{\varepsilon}} \right)^{1/q} \right] \right\} \left( \frac{\hat{\sigma}}{\mu_0} \right)^p, \quad (18)$$

on the other hand:

$$\frac{\sigma}{\mu} = \frac{\sigma_a}{\mu_0} + \left\{ 1 - \left[ \frac{kT}{g_0 \mu b^3} \ln \left( \frac{\dot{\varepsilon}_0}{\dot{\varepsilon}} \right)^{1/q} \right] \right\}^{1/p} \frac{\hat{\sigma}}{\mu_0}, \quad (19)$$

where  $0 < p \leq 1$  and  $1 < q \leq 2$ . Equation (18) and (19) represent the form of the “yield stress” equation that will be used in MTS formulations going forth – replacing the simplified Equation (1). In the form of Equation (13):

$$\frac{\sigma}{\mu} = \frac{\sigma_a}{\mu} + s(\varepsilon, T) \frac{\hat{\sigma}}{\mu_0}, \quad (20)$$

where:

$$s(\varepsilon, T) = \left\{ 1 - \left[ \frac{kT}{g_0 \mu b^3} \ln \left( \frac{\dot{\varepsilon}_0}{\dot{\varepsilon}} \right)^{1/q} \right] \right\}^{1/p}. \quad (21)$$

The values of the coefficients  $p$  and  $q$  have been set  $p = 1/2$ ,  $q = 3/2$  [5].

Equation (18) can be written as:

$$\left( \frac{\sigma - \sigma_a}{\mu} \right)^{1/2} = \left\{ 1 - \left[ \frac{kT}{g_0 \mu b^3} \ln \left( \frac{\dot{\varepsilon}_0}{\dot{\varepsilon}} \right)^{2/3} \right] \right\} \left( \frac{\hat{\sigma}}{\mu_0} \right)^{1/2}. \quad (22)$$

Equation (22) can be written after taking into account the values given in the task:

$$\left(\frac{\sigma - 100 \cdot 10^6}{\mu}\right)^{1/2} = \left\{ 1 - \left[ \frac{k \cdot T}{g_0 \cdot b^3 \cdot \mu} \ln\left(\frac{10^8}{\dot{\epsilon}}\right)^{2/3} \right] \right\} \left(\frac{\hat{\sigma}}{\mu_0}\right)^{1/2},$$

$$\left(\frac{\sigma - 100 \cdot 10^6}{\mu}\right)^{1/2} = f \left[ \frac{8 \cdot 10^5 \cdot T}{\mu} \ln\left(\frac{10^8}{\dot{\epsilon}}\right)^{2/3} \right]. \quad (23)$$

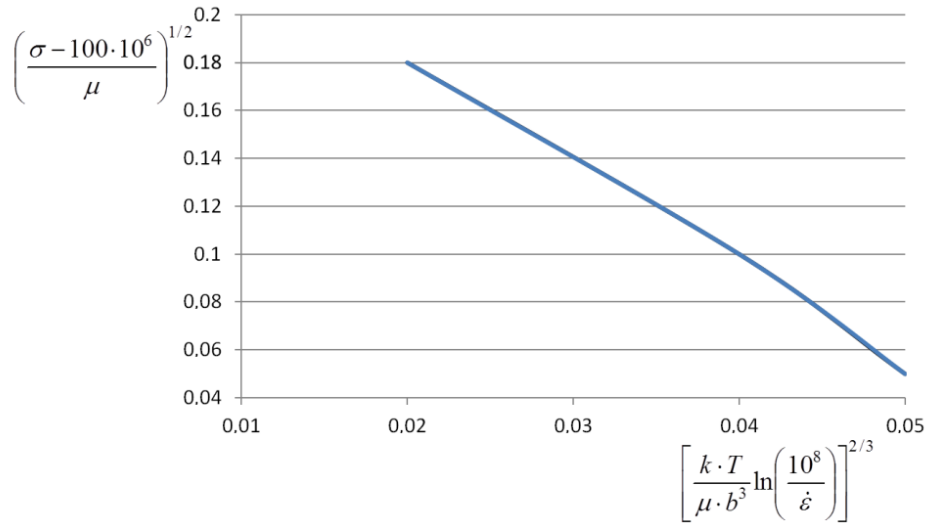


Fig. 5. The dependence between the yield stress of molybdenum and the temperature with strain rate on the basis of the Tab. 1 and dependence (23)

Figure 5 shows the dependency between the yield stress of molybdenum change and the strain rate with the temperature taking into account the activation stress and other parameters.

### 3. Summary and conclusions

Example molybdenum samples which have been exposed to stretching depending on the temperature and strain rate showed a significant change of the strength parameters. It should be noted that values of the modulus of elasticity has not changed significantly along with the temperature change. Based on the dislocation theory, an additional increase strength of the material due to interaction of dislocations with grain boundaries occurs.

The resulting stress is an athermal stress. A wealth of experimental data is available on yield stress as a function of test temperature and strain rate.

On the basis of equation (1) which determines the dependence of yield stress from the temperature and strain rate there was, determined detailed form of the equation (19). Equation (19) includes not only mechanical parameters but also the structural ones.

Therefore, it is possible to describe the yield stress from the temperature, strain rate and mechanical threshold stress very precisely. Introducing the concept of mechanical threshold stress (MTS) allows following the variables of the state and determining the current value of the material effort.

The obtained results, are allowing the prediction even for the stresses that were not described, because of being outside the measurement scope, which makes them significant.

Evolution of the threshold stress characterizing the stored dislocation density was described using a phenomenological physics basis.

Three internal state variable have been used to have a deeper understanding of the operative deformation mechanisms (and the obstacle populations opposing dislocation motion).

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