

INFLUENCE OF GRAIN BOUNDARY SEGREGATION, DEFORMATION TEMPERATURE ON STRENGTH IN ULTRAFINE-GRAINED Al AND Ti ALLOYS

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Abstract. The presented work considers one of the promising ways of enhancement of strength in ultra fine-grained (UFG) metal materials produced as a result of application of severe plastic deformation techniques. Mathematical modeling showed that structure design in UFG Al and Ti alloys enabled significantly increasing their strength. By introducing impurity atoms with fixed concentration in the matrix and subjecting material to relevant processing, one can form UFG structures with a high strength including at elevated temperatures.

1. INTRODUCTION

It is known that significant structure refinement occurs as a result of large plastic deformations [1]. The microstructure is characterized by mainly low-angle boundaries that divide cells and blocks of cells. The method of severe plastic deformations (SPD) that implies achievement of large plastic strains ($\epsilon > 1 \div 10$) under high applied pressures of several GPa results in formation of UFG structures and even nanocrystalline states with mainly high-angle non-equilibrium grain boundaries [2]. High pressure torsion (HPT) and equal channel angular pressing (ECAP) are main SPD techniques [2]. It was stated that not only grain size but also defect structure of grain boundaries (GB) could influence the strength properties of metals [3]. The role of GBs as dislocation sources and sinks in UFG materials enlarges. Non-equilibrium state of GBs, high dislocation density in GBs and lack of dislocations in grain interiors are typical of such materials. Specific structural arrangement of grains creates conditions for sink of impurity atoms in GB areas. Dislocations in GBs are found in solid solution with enhanced concen-

tration C_0 of impurity atoms. This process can be intensified at temperature or mechanical impact from outside. There is force interaction between a dislocation and a cloud of impurity atoms, which depends on the concentration C_0 , the size mismatch factor ϵ between the matrix and impurity atoms, and the temperature T . The higher are the values of C_0 and ϵ , the higher is the interaction force. Impurity atoms forming grain boundary segregations pin grain boundary dislocations and increase the material strength. The temperature increase contributes to dissipation of the cloud and, therefore, reduction of the force interaction.

The authors of the works [4,5] analyzed the causes of experimentally observed high values of the yield stress, which deviate from the Hall-Petch law to higher stresses, in alloy 1570 (Al – base, Mg – 5.7, Sc – 0.32, Mn – 0.4, wt.%) subjected to HPT at different temperatures [6] and in Ti Grade 4 (Ti – base, C – 0.052, O – 0.34, Fe – 0.2, N – 0.015, wt.%) subjected to ECAP and subsequent annealing [7]. The experimental studies of the samples structure revealed segregations of impurity atoms along GBs. The segregations play an important role

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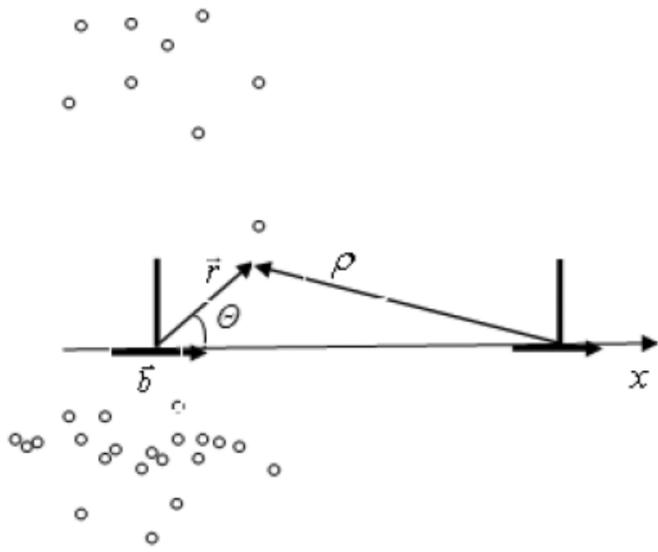


Fig. 1. Motion of an edge dislocation for the distance x from a cloud of impurity atoms.

in formation of the mentioned super-strength states [6,7].

The aim of this work is to model pinning of edge dislocations by a cloud of impurity atoms in Al- and Ti-based alloys depending on the temperature T and factor of size mismatch ε .

2. THE DISLOCATION PINNING BY ATMOSPHERES OF IMPURITY ATOMS

As it is known, the force acting on a dislocation during its motion for the distance x from the frozen cloud of impurity atoms (Fig. 1) is determined in the following way:

$$F = \tau_s bL = \frac{\partial W}{\partial x}, \quad (1)$$

where W – the energy of interaction of an edge dislocation with a cloud of impurity atoms, τ_s – the stress of edge dislocation pinning, b – the Burgers vector value, L – the dislocation length.

Table 1. Atomic radius values of investigated elements.

Chemical element	Mg	Ce	Be	Al
Atomic radiuses, pm	160	181	112	143

Table 2. Atomic radius values of investigated elements that form limited solid solutions with Ti.

Chemical element	Th	Be	Ni	Fe	Pd	Ti
Atomic radiuses, pm	180	112	124	126	137	147

The energy of interaction of an edge dislocation with an impurity atom w with account of stress tensor components in the gradient theory of elasticity [8–10] can be written as

$$w = \beta \left[\frac{1}{r} - \frac{K_1\left(\frac{r}{\sqrt{s}}\right)}{\sqrt{s}} \right] \sin \Theta, \quad (2)$$

where $\sqrt{s} \approx a/4$ – the gradient coefficient for an edge dislocation, a – the crystalline lattice parameter, $\beta = (4/9)a^3\varepsilon Gb(1+\nu)/(1-\nu)$, $\varepsilon = (R_s - R_a)/R_a$, R_a – the matrix atom radius, R_s – the impurity atom radius, G – the shear modulus, ν – the Poisson coefficient, r – the radius-vector of an impurity atom with its origin in the dislocation nucleus, Θ – the angle between the Burgers vector and radius-vector r . In the direction of the Burgers vector the angle $\Theta = 0$ (Fig. 1). $K_1(r/\sqrt{s})$ – the modified Bessel's function of the second type of the first order. The extreme value of dimensionless interaction energy $\tilde{w} = w\sqrt{s}/\beta$ determined for $\theta = 3\pi/2$ and $\theta = \pi/2$ is achieved at $y_0 \approx 1.115$, where $y = r\sqrt{s}$ [10]. When $y = y_0$, the binding (attraction) energy at $\theta = \pi/2$ reaches the maximum value, while $\beta > 0$, at $\theta = \pi/2$ in case $\beta < 0$. The substitution atoms with $R_s > R_a$ and all interstitial atoms are attracted to the area under the edge of an extraplane, the substitution atoms with $R_s < R_a$ are attracted to the area above the edge of an extraplane.

Uniform distribution of the concentration of point defects around a dislocation is described by the ratio

$$C_d = C_{d0} \exp\left(-\frac{w}{k_B T}\right), \quad (3)$$

where k_B – the Boltzmann coefficient, T – the temperature, C_{d0} – the concentration of point defects far from a dislocation. The total interaction energy W between a dislocation and a cloud of impurity atoms during dislocation motion from the frozen cloud for the distance x equals

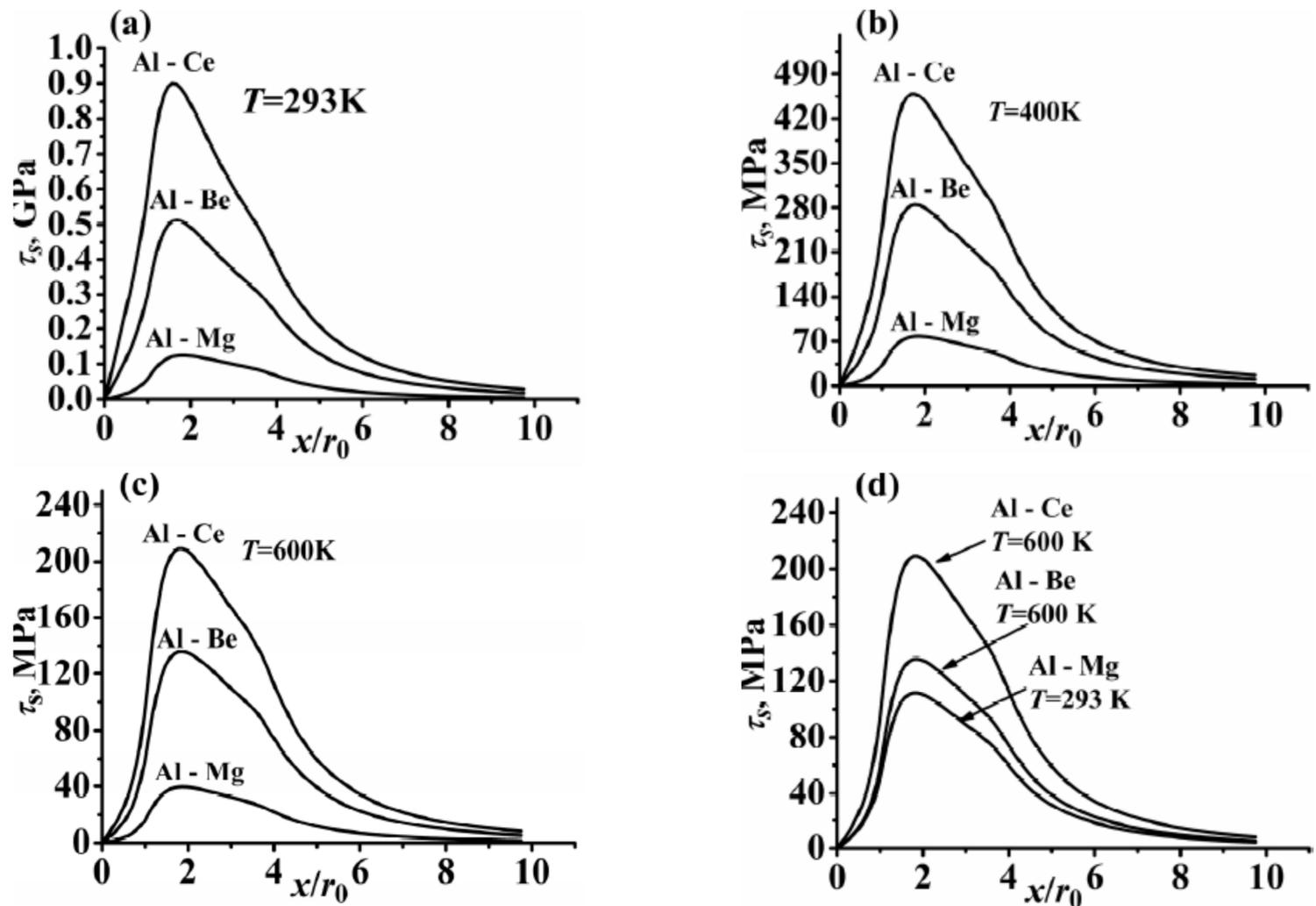


Fig. 2. Stress of edge dislocation pinning by a cloud of Mg, Be, Ce atoms at $T = 293\text{K}$ (a), at $T = 400\text{K}$ (b), at $T = 600\text{K}$ (c). Stress of edge dislocation pinning by a cloud of Mg atoms at $T = 293\text{K}$ and by a cloud of Be and Ce atoms at $T = 600\text{K}$ (d). $C_0 = 98.37 \times 10^{26} \text{ m}^{-3}$, $r_0 \approx 1.45b$.

$$W = L\beta \int_{r_0}^{\infty} \int_0^{2\pi} (C - C_{d0}) \left[\frac{1}{\rho} - \frac{K_1\left(\frac{r}{\sqrt{s}}\right)}{\sqrt{s}} \right] \frac{r \sin \Theta}{\rho} r dr d\Theta, \quad (4)$$

where $\rho = \sqrt{r^2 + x^2 - 2rx \cos \Theta}$.

According to Eq. (1), the dependence of edge dislocation pinning force on the displacement value x has the view

$$\frac{F\sqrt{s}}{L} = 4\beta C_{d0} \int_{r_0}^{\infty} \int_0^{\pi} sh \left[\frac{\beta}{kT} \left(\frac{1}{r} - \frac{K_1\left(\frac{r}{\sqrt{s}}\right)}{\sqrt{s}} \right) \sin \Theta \right] \times \left\{ \frac{\sqrt{s}r^2 (x - r \cos \Theta) \sin \Theta}{(x^2 + r^2 - 2rx \cos \Theta)^2} - \frac{r^2 Q(x) (x - r \cos \Theta) \sin \Theta}{(x^2 + r^2 - 2rx \cos \Theta)} \right\} dr d\Theta, \quad (5)$$

$$Q(x) = \frac{K_0\left(\frac{\rho}{\sqrt{s}}\right)}{2\sqrt{s}} + \frac{K_1\left(\frac{\rho}{\sqrt{s}}\right)}{\rho}.$$

$K_0(\rho/\sqrt{s})$ - the modified Bessel's function of the second type of zero order.

Integration with the variable r is conducted in the range from the size of a dislocation nucleus r_0 to r . There was accepted a value $r = r_0 + 2.774a$ in calculation, that does not impact the maximum meaning of the value τ_s .

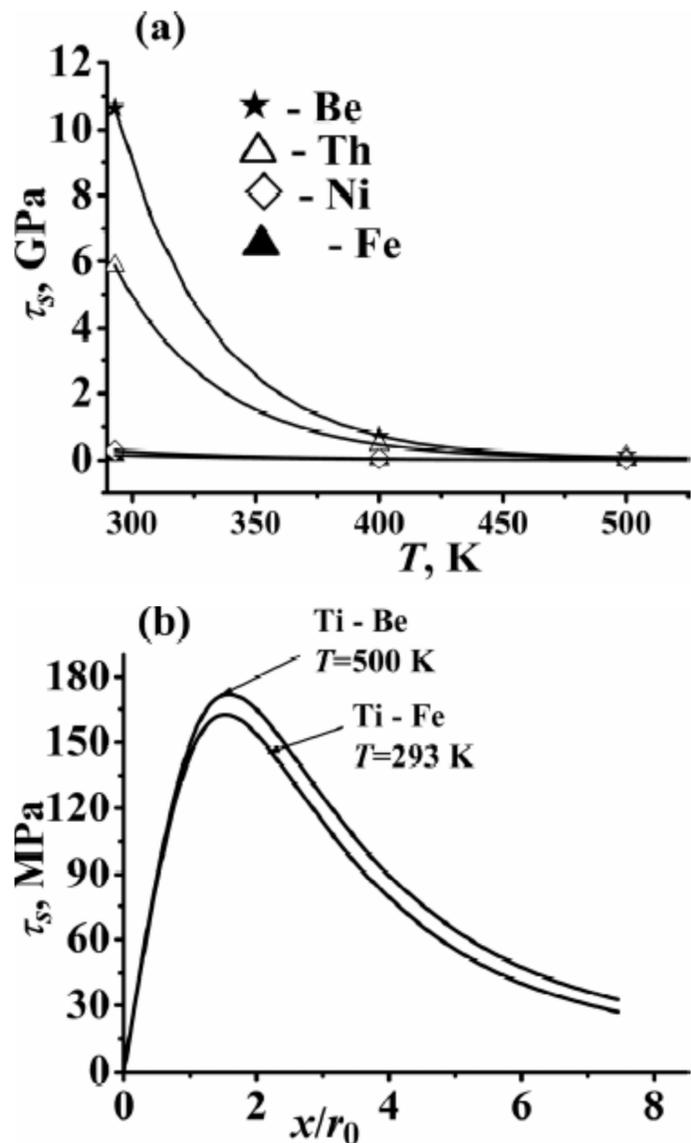


Fig. 3. The temperature dependences of stress of edge dislocations pinning by clouds of impurity atoms of Be, Th, Ni, Fe (a). Stress of edge dislocation pinning by a cloud of Fe atoms at $T = 293$ K and by a cloud of Be atoms at $T = 500$ K (b). $C_0 = 97.85 \times 10^{24} \text{ m}^{-3}$, $r_0 = 1.115a/4$.

As the authors demonstrated in [6], precipitation of Mg atoms from the solid solution into the GB area about 3 nm wide [6] could take place during processing of hot-pressed alloy Al 1570 (Al – base, Mg – 5.7, Sc – 0.32, Mn – 0.4, wt.%) annealed at 380 °C for 2 hours (coarse-grained (CG) state) by high pressure torsion (HPT) at room temperature (RT) (state UFG 1) and at temperatures of 100 °C (state UFG 2) and 200 °C (state UFG 3). The Mg atoms precipitate in different quantities depending on the processing temperature. The deviations from the Hall-Petch law to higher stresses were stated. The work [4] presents the results of numerical modelling of regularities of plastic deformation of the Al 1570 alloy in different states, which are observed experimentally. It was revealed that ultra-high-strength states of samples were conditioned by pinning of dislocations by Mg atoms diffused into the GB area during HPT. The concentration of impurity atoms away from the dislocation C_{o0} was accepted equal to the enhanced concentration in the segre-

gation C_0 ($C_{o0} = C_0$), as at a distance of 3 nm from a dislocation, impurity atoms feel the dislocation field weakly. Therefore, the concentration of impurity atoms C_{o0} is little different from the concentration in the segregation C_0 [8].

Let us assume that the same quantity of Be or Ce atoms precipitated instead of Mg atoms in the GB area during processing by SPD techniques. Table 1 lists the values of the radiuses of their atoms. The contribution of the stress of dislocation pinning τ_s by impurity atoms at one and the same temperature and concentration C_0 in the alloy yield stress will differ considerably depending on the size R_s of corresponding atoms. For example, substitution of Mg atoms with Be atoms in the Al matrix enables enhancing the stress of dislocation pinning at RT ≈ 4.1 times (Fig. 2a), at 400K ≈ 3.7 times (Fig. 2b), at 600K ≈ 3.4 times (Fig. 2c). The stress of dislocation pinning by Be atoms at 600K is even higher the stress of pinning by Mg atoms at RT (Fig. 2d).

If we assume that it was Ce atoms and not Mg ones that precipitated in GB, the stress of dislocation pinning at equal values of C_0 and T can be increased ≈ 7.2 , ≈ 5.9 , ≈ 5.3 times at the mentioned temperatures respectively (Fig. 2). The stress of dislocation pinning by Ce atoms at 600K is higher than the stress of dislocation pinning by Mg atoms at RT (Fig. 2d). When calculating the stress of edge dislocation pinning in Al alloys the following parameters $\nu = 0.32$, $b = 0.286 \text{ nm}$, $G = 25.5 \text{ GPa}$, $a = 0.404 \text{ nm}$ have been used.

Precipitation of O and C atoms from the solid solution in the grain boundary area was observed also in UFG Ti Grade-4 (Ti–base, C–0.052, O–0.34, Fe–0.2, N–0.015, wt. %) samples processed by ECAP and subsequent annealing for 6 hours [7]. Precipitation of impurity atoms of N was negligible. However, in this case the stresses of dislocation pinning by impurity atoms precipitated along GBs did not significantly impact the yield stress of samples [5]. Pinning of edge dislocations by Fe atoms considerably influenced the yield stress, which resulted in formation of high-strength states deviating from the Hall-Petch law [5]. Substitution of Fe atoms in Ti samples by other elements, which differ in the size mismatch factor, can lead to more pronounced ultra-high-strength states. We shall consider some elements that can form limited solid solutions with Ti (Table 2).

Fig. 3a displays the temperature dependences of stress of edge dislocations pinning by clouds of impurity atoms of Be, Th, Ni, Fe. Under the appropriate choice of the size mismatch factor ε , the stress of dislocation pinning by atoms at elevated

temperatures can be higher than that at room temperature. For example, the stress of dislocation pinning by a cloud of Be atoms at 500K is higher than the stress of pinning by Fe atoms at RT (Fig. 3b).

When calculating the stress of edge dislocation pinning in Ti alloys the following parameters $\nu = 0.32$, $b = 0.295$ nm, $G = 41.0$ GPa, $a = 0.296$ nm have been used.

By subjecting the alloys with the matched factor of size mismatch and corresponding concentration to SPD, by fabricating the required structures, one can significantly increase their yield stress and produce materials, which would not lose high strength even at high temperatures.

3. CONCLUSIONS

In summary, the results of studies conducted by mathematical modeling showed that by increasing the size mismatch factor via selection of an element with the corresponding atom radius, one can significantly enhance the contribution of stress of dislocation pinning by impurity atoms in the yield stress of the investigated alloys. The pinning stresses at elevated temperatures in the considered model alloys are even higher than those at RT in Ti alloy with Fe and Al alloy with Mg. Application of SPD techniques allows producing UFG materials with non-equilibrium GBs, which creates possibility for designing light-weight high-strength materials due to dislocation pinning by impurity atoms in GBs. Such materials can be used in different areas of science and engineering, where the requirements to the strength-to-weight ratio retain actual even at elevated temperatures.

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