Strengthening Induced by Grain Boundary Solute Segregations in Ultrafine-Grained and Nanocrystalline Alloys: a Brief Review

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Abstract. The experimental data, computer simulations and analytical models describing strengthening mechanisms acting in nanocrystalline and ultrafine-grained alloys containing grain boundary solute segregations are briefly reviewed. We demonstrate the important role of grain boundary solute segregation in strength enhancement of ultrafine-grained alloys. We show that these segregations allow reaching yield strength exceeding one predicted by the Hall-Petch dependence. Available experimental and theoretical data indicate that strengthening induced by grain boundary solute segregations is achieved by either suppressing dislocation emission from GBs or hampering dislocation slip through grain interiors.

Nanocrystalline and ultrafine-grained metals and alloys are the subject of intensive scientific research as they often demonstrate outstanding mechanical properties [1-8]. It is known that the yield strength is related to the mean grain size via the classic Hall–Petch relationship (see recent reviews [9-13]). Over past decade a number of ultrafine-grained (UFG) and nanocrystalline (NC) alloys have been engineered [14-20] using severe plastic deformation (SPD) that exhibit considerably higher strength than the Hall-Petch relationship predicts. The nature of this enhanced strength is a matter of debate. It is often attributed, in particular, to the experimentally detected [14-22] segregations of solute elements at grain boundaries (GBs). In this work we briefly review recent experimental and theoretical data concerning this enhanced strength of UFG and N alloys containing GB solute segregations.

Authors of experimental works [16-19] reported ultra-high strength close to 1 GPa for the SPD-processed Al alloys 1570, 5083, 7475, and 7075. For example, in the Al alloy 1570 with a mean grain size of 100 nm, the yield strength is approximately 200 MPa higher than the Hall-Petch relationship predicts for an alloy with the same grain size and chemical composition (Fig. 1 [16]). Dotted line in Fig. 1 shows projected Hall-Petch dependence for Al alloy 1570 (for details, see [16]). The common feature that all these alloys share is the formation of segregations of solute atoms at GBs [14-19]. Fig. 2a shows atom probe tomography image of Al alloy 5083 specimen [17]. Mg atoms segregations are observed at certain locations on the grain boundaries (Fig. 2b), which is believed to be the reason of these Al alloys excellent strength.

Strength enhancement attributed to solute segregations at GBs has also been documented in coarse-grained [23] and UFG [14,18-20] carbon steels, a nanocrystalline TWIP steel [22], an UFG Al-Mg-Si alloy [21], as well as in nanocrystalline Cu alloys [24-26], an Al–Cu alloy [27] and Cu-Ta alloy [28]. The underlying mechanisms of this segregation-induced strength enhancement remain a matter of debate.

For example, Zhang et al. [26] measured a considerable increase in hardness, tensile ductility and fatigue lifetime of nanocrystalline Cu thin films after the addition of Zr. Experimental results showed that the Cu–0.5 at.% Zr film exhibited the highest hardness, largest duc-
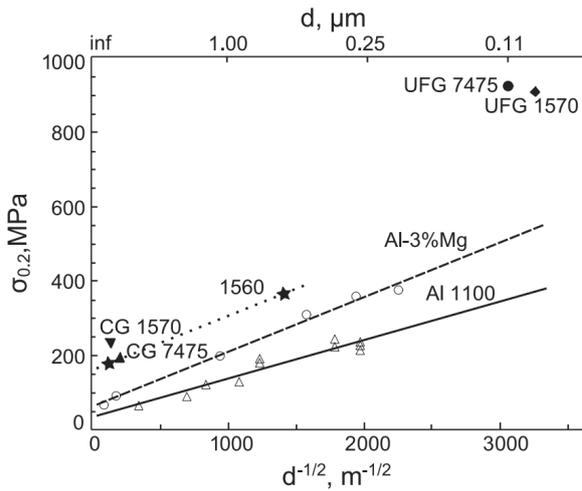
Fig. 1. The Hall-Petch relation for the Al alloys: 1100, Al–3%Mg and data on the yield stresses of Al alloys: 1560, 1570, 7475. Dotted line is the projected Hall-Petch relation for 1570 alloy. Reproduced from [16] with permission. Copyright (2010), Elsevier.

tility and longest fatigue lifetime, which are increased by 120%, 80%, and above an order of magnitude, respectively, in comparison with its pure Cu counterpart. They found that at 0.5 at.% Zr content the film exhibited the yield strength of 1600 MPa, while the combined effect of the GB and nanotwin strengthening predicted the yield strength of 1100 MPa. They attributed the discrepancy to the formation of GB Zr segregations. They suggested that Zr segregation at GBs significantly reduce the GB energy, which suppresses GB migration and other GB activities and hence increases the strength.

Chang and Hong [29] and Valiev et al. [16] assumed that segregation-induced strengthening is associated with a decrease in the activation volume for plastic flow experimentally documented [29] in a Zr-Nb alloy after

the addition of sulfur segregated along GBs. They defined this activation volume V_a as:

$$V_a = kT \partial \ln \dot{\gamma} / \partial \tau = nkT \ln(\dot{\varepsilon})_1 / (\dot{\varepsilon})_2 / (\sigma_1 - \sigma_2), \quad (1)$$

where τ is the shear stress, n is the Taylor factor (taken equal to 4), k is the Boltzman constant, $\dot{\gamma}$ is the shear strain rate, σ_1 and σ_2 are the applied shear stresses at the normal strain rates $(\dot{\varepsilon})_1$ and $(\dot{\varepsilon})_2$. Experiments showed that the activation volume V_a decreased from $110b^3$ to $80b^3$ where b is the Burgers vector with the addition of 300 ppm sulphur at room temperature. Chang and Hong [29] discussed actual mechanisms leading to the decrease of activation volume and suggested that sulfur atoms pin segments of dislocations emitted from GBs thus affecting the activation length of dislocations. But no numerical model allowing calculating the effect on yield strength was suggested.

Borovikov et al. [30] suggested that segregation-induced strength enhancement is associated with a decrease of the number of active GB dislocation sources. Their suggestion is based on the results of their computer simulations of deformation of nanocrystalline Ag containing GB Cu segregations [30]. The simulations revealed that the yield strength of nanocrystalline Ag (containing GB Cu segregations) first increases and then decreases with an increase in Cu concentration (Fig. 3) and demonstrated the existence of GB and triple junction dislocation sources. The simulations also showed that a part of these sources (that could be treated as GB and triple junction dislocation segments) is pinned (deactivated) by Cu segregations. Since some favorable dislocation sources are inactive, dislocations are emitted from less favorable sources (activated at a higher stress), which results in an increase in the yield strength of the nanocrystalline solid. At the same time, at high enough average Cu concentration, the concentration of Cu in Cu segregations located at dislocation sources
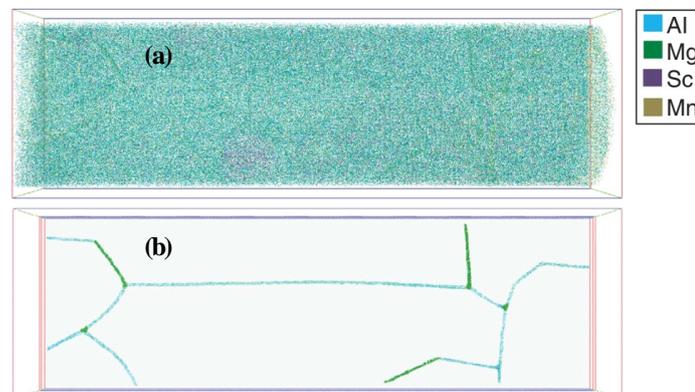

Fig. 2. (a) Atom probe tomography image of NH-5083 alloy. (b) The image revealing the grain-boundary locations in a thin ~1-nm-thick slice of data. Solute segregations are observed at certain locations on the grain boundaries. Reproduced from [17] with permission. Copyright (2010), Macmillan Publishers Limited.
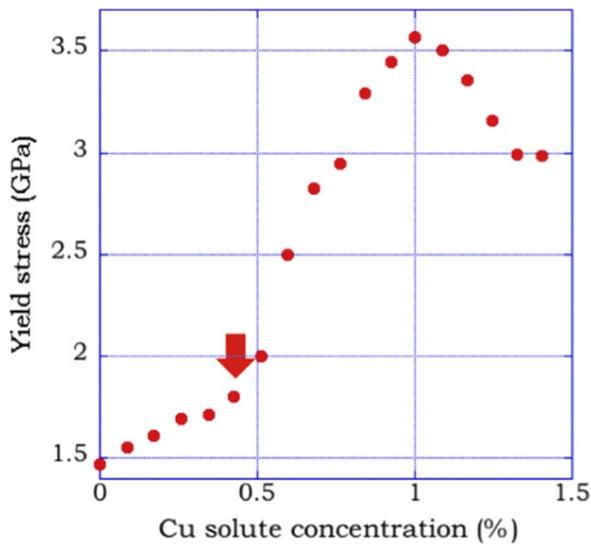
Fig. 3. The dependence of the yield stress of the Ag-Cu alloy on solute concentration (at.%). Reproduced from [30] with permission. Copyright (2018), Elsevier.

also becomes very high, resulting in the creation of very high elastic stresses at segregation boundaries. These stresses appear to be sufficiently high to induce dislocation nucleation at segregation boundaries, which serve as new dislocation sources. The formation of new segregation-induced dislocation sources reduces the yield strength of nanocrystalline Ag-Cu alloys at high Cu concentrations.

In contrast to the models discussed above that explain the enhanced strength of metallic alloys containing GB solute segregations by the restraining effect of the segregations on dislocation nucleation at GBs, Turlo and Rupert [31] assumed that strength enhancement is

also determined by the effect of segregations on dislocation propagation across grains. Their assumption is based on the results of their atomistic simulations of plastic deformation of Cu bicrystals containing GB segregations of Zr. They compared propagation of dislocations in structures with three different types of GBs (Fig. 4). Namely, clean grain boundaries (CGBs) without any solute atoms, GBs containing periodic distribution of solute atoms or, as they call it, ordered grain boundary complexion (OGBC) and amorphous intergranular films (AIF), characterized by very high concentration of solute atoms. According to the simulations [31], the critical stress for dislocation nucleation at GBs decreases, and the critical stress for dislocation propagation across a grain increases owing to the presence of Zr segregations. Comparing their simulation results with this experimental data [24], Turlo and Rupert [31] concluded that the rate-limiting deformation mechanism in nanocrystalline Cu-Zr alloys is dislocation pinning by GB segregations during dislocation propagation.

The results of other computer simulations [32-35] indicate that the strengthening effect of GB segregations depends strongly on the lattice mismatch of solute and matrix atoms as well as on the plastic deformation mechanisms. For instance, Vo et al. [34] revealed in the simulations a considerable increase in the yield strength of nanocrystalline Cu alloys due to GB solute segregations, which scaled linearly with the lattice mismatch of the solute and matrix atoms (Fig. 5). This result was later confirmed experimentally [25].

Babicheva et al. [33] demonstrated in the molecular dynamics simulations a moderate increase of the yield strength of nanocrystalline Al due to GB Co segregations
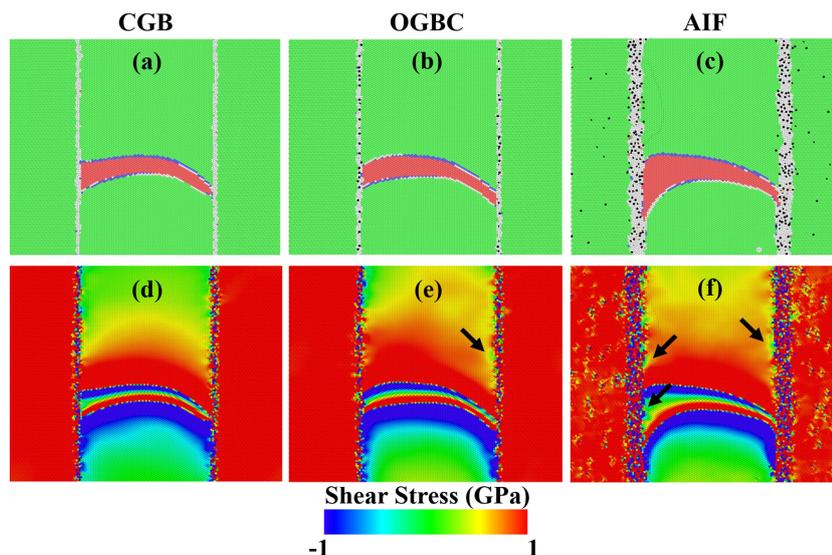

Fig. 4. (a–c) Local atomic structure and (d–f) atomic shear stress distribution during dislocation propagation simulations in Cu-Zr alloy at 3% applied shear strain. Black arrows denote local regions of low stress. Reproduced from [31] with permission. Copyright (2018), Elsevier.
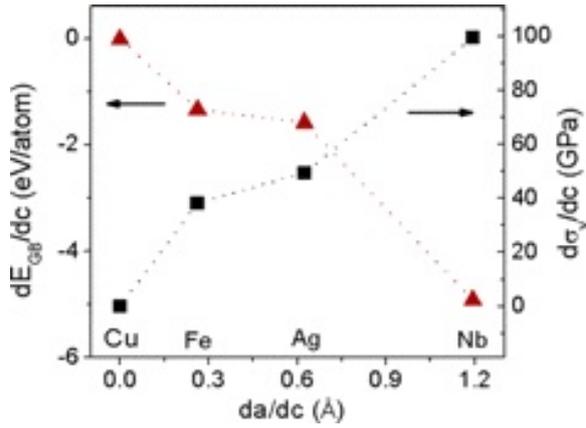
Fig. 5. Linear relationships between lattice mismatch of solute and matrix atoms vs GB energy and yield strength of nc Cu samples. Reproduced from [34] with permission. Copyright (2011), Elsevier.

and the absence of the strengthening effect for Mg segregations. Moreover, earlier atomistic simulations [35] showed that GB Pb segregations reduce the yield strength of nanocrystalline Al. In both cases, the simulations demonstrated that room-temperature deformation of nanocrystalline Al (containing Mg or Pb segregations) occurs via GB sliding or GB sliding coupled with GB migration. Therefore, one can conclude that although GB Pb segregations hamper lattice dislocation slip, these can promote GB sliding, and enhanced GB sliding leads to a decrease in the yield strength.

Bobylev et al. [36] recently developed theoretical model explaining experimentally observed enhanced strength of UFG alloys containing GB segregations. Unlike previous models it takes into account not only
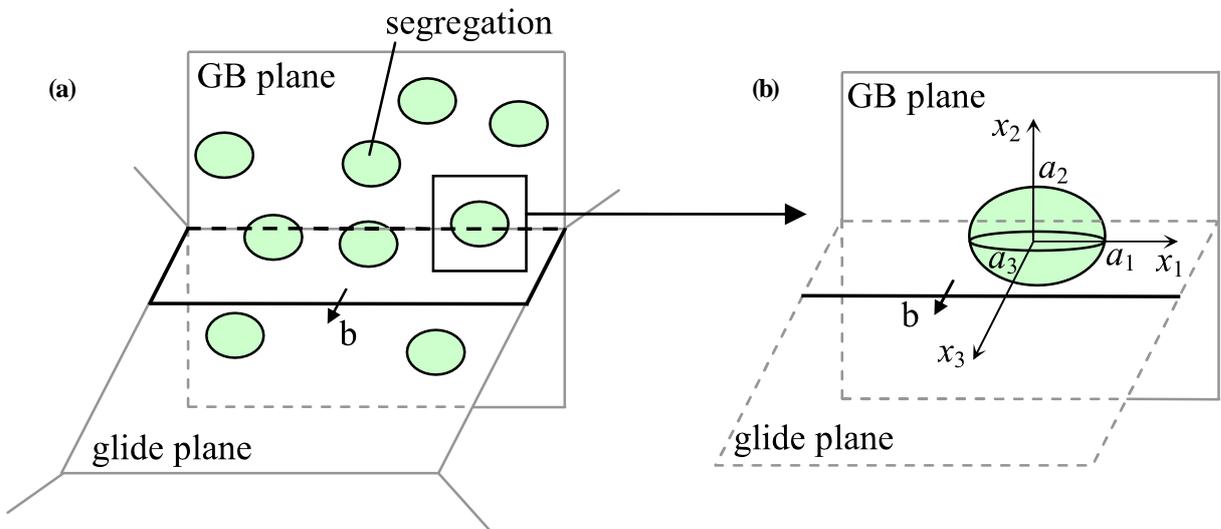
concentration of the solute but also a shape and size of segregations. In the framework of proposed model segregations were treated as the coherent ellipsoidal inclusions dispersed in the random way over GBs (Fig. 6a). The ellipsoidal shape (characterized by half axes a_1, a_2, and a_3; see Fig. 6b) of the inclusions was chosen as a good approximation for a range of actual segregation shapes (spheres, ellipsoids, plates) observed, in particular, in UFG Al alloys [14-19]. The difference between the solute concentrations c_s and c_m inside and outside the inclusions, respectively, leads to a change of the lattice parameter a_{ss} of the inclusions:

$$a_s \approx a_m + 100(c_s - c_m)\Delta a, \tag{2}$$

where a_m is the matrix lattice parameter and Δa is the change of the lattice parameter of the alloy associated with an increase of the solute concentration by 0.01 (that is, by 1 at.%). As a result, an internal strain (eigenstrain) is created inside the inclusions. Assuming the dilatational character of eigenstrain, the eigenstrain tensor ε_{ij}^* is written as

$$\varepsilon_{ij}^* = \varepsilon^* \delta_{ij}, \tag{3}$$

where $i,j = 1,2,3$, δ_{ij} is the Kronecker delta, and ε_{ij}^* is the lattice mismatch between the inclusion and the matrix, defined as

$$\varepsilon^* = \frac{a_s - a_m}{a_m}. \tag{4}$$

In the exemplary case of Al alloy 1570 the value of ε^* was found to be ~0.01, which is low enough to provide the coherency of the matrix–inclusion interface.

Fig. 6. (a) Grain boundary with randomly dispersed segregations (green ovals) and dislocation that nucleated at the same grain boundary. (b) Magnified inset showing a single ellipsoidal inclusion with a dislocation line in its vicinity. Reproduced from [36] with permission. Copyright (2019), Elsevier.
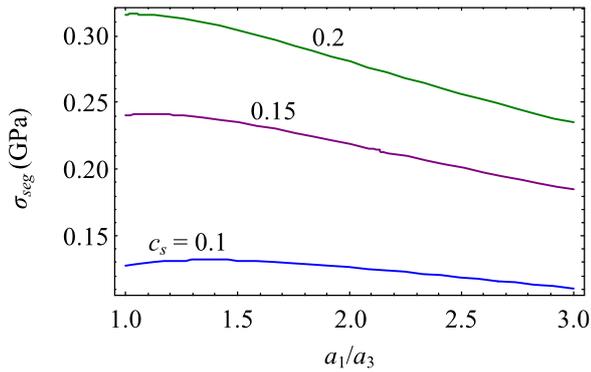
Fig. 7. Dependences of the segregation contribution σ_{seg} to the yield stress of Al alloy 1570 on the segregation aspect ratio a_1/a_3, calculated under the assumption that the average solute concentration $\overline{c}_{gb}$ in the GB layer is constant, for c_m=0.064, $\overline{c}_{gb}$ = 0.073, c_s=0.1, 0.15, and 0.2.

Due to internal strain each ellipsoidal inclusion produces an elastic stress field that creates forces acting on dislocation segments in its vicinity and can prevent their emission from GBs by pinning them immobile. To overcome these forces external stress must by increased by some value σ_{seg}. Using theory of dislocation and inclusions Bobylev et al. [36] calculated dependences (Fig. 7) of the value σ_{seg} on aspect ratio a_1/a_3 (it was assumed $a_1 = a_2$) of the inclusion in the exemplary case of Al alloy 1570 with Mg GB segregations using following values of parameters (corresponding to experimentally measured [15, 16] values): $c_m = 0.064$, $\overline{c}_{gb} = 0.073$, $a_3 = 5$ nm, $c_s = 0.1$, 0.15, and 0.2, where $\overline{c}_{gb}$ – average solute concentration inside GB (assumed to be constant). From Fig. 7 it is seen that in the case of the constant concentration $\overline{c}_{gb}$ stress σ_{seg} reaches maximum at low aspect ratio values a_1/a_3 (approximately 1.0–1.4 depending on concentration c_s) and then decreases. This means that small spherical or nearly spherical segregations provide higher strengthening compared to elongated ellipsoidal segregations. Also Fig. 7 shows that increase in concentration c_s leads to higher values of σ_{seg}. The model [36] allows making a conclusion that maximum strengthening due to GB solute segregations is achieved when solute atoms are accumulated in small concentrated clusters as opposed to spreading uniformly over GBs. As it follows from Fig. 7 the value of σ_{seg} at $c_s \approx 0.15$ is close to experimentally measured strengthening of alloy 1570 equal to ~200 MPa [16]. Thus proposed model agrees relatively well with the experiment.

In conclusion, the results of experiments and simulations demonstrated that GB solute segregations tend to increase the yield strength of UFG and NC alloys. Experimental and theoretical data points to two possible mechanisms of GB segregation induced strength enhancement: (1) suppression of dislocation emission from GBs and (2) suppression of dislocation slip through grain by pinning or elastic interaction between dislocations and GB segregation. It seems that both types of mechanisms are possible and their effectiveness depends on the crystal structure and chemical composition of material. The suppression of dislocation emission most likely requires realization of specific atomic structures, so this mechanism is unlikely to be universal and effective in any type of material. Similarly, suppression of dislocation slip should be more pronounced in the materials where solute atoms produce noticeable lattice parameter change, thus producing relatively high elastic stresses interacting with moving dislocations. At the same time, if solute atoms do not affect lattice parameter this mechanism should be ineffective. Recent findings by Bobylev et al. [36] indicate that if strengthening is controlled by elastic interaction between GB solute segregations and lattice dislocations then the maximum strengthening of an alloy is achieved by the formation of GB solute segregations in the form of small concentrated clusters, instead of homogeneous distribution of solutes over GBs.

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