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Effect of grain boundary segregation on the deformation mechanisms and mechanical properties of nanocrystalline binary aluminum alloys

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ABSTRACT

The deformation mechanisms of nanocrystalline (NC) pure Al and NC Al–Co and Al–Mg binary alloys are studied via molecular dynamics simulation. The alloying elements are either segregated to grain boundaries (GB) or distributed randomly as solute. It is revealed that a shear deformation of the pure Al is associated with the GB sliding (GBS) and simultaneous their migration (GBM). GB segregations can significantly alter the mechanisms of plastic deformation. Mg atoms in GBs of the Al–Mg alloy lead to GBS which is accompanied with GBM and a grain growth, while the deformation process of the corresponding alloy with the random distribution of Mg is close to that for pure Al. Unlike Mg, GB segregations of Co atoms detain both GBS and GBM and result in a higher strength of the Al–Co alloy. On the contrary, the strength of the alloy with the Co atoms distributed randomly is very low due to the structure amorphisation leading to the ease of plastic flow. The details of the GBS and GBM processes are further studied for tilt bi-crystals of Al and Al–Co and Al–Mg systems with the alloying atoms being either segregated to the GB or dissolved. It is found that the results for the bi-crystals are in line with those for the NC materials. Overall, GB segregation can strongly influence the response of NC alloys to thermomechanical treatment by affecting such very important mechanisms of plastic deformation in NC metallic materials as GBS and GBM.

1. Introduction

Bulk ultra-fine grain (UFG) and nanocrystalline (NC) metals have great potential in many applications due to their high ultimate strength and the ability to demonstrate superplasticity effect [1–11]. However, the usage of such materials is limited by their low ductility at ambient conditions due to premature crack initiation along grain boundaries (GBs) that would eventually lead to their fracture [12,13]. Another weak point of the bulk NC materials, especially for pure metals, is their low thermal stability. During deformation and/or aging at elevated temperatures, a high non-equilibrium material with a large density of GBs transforms to a more stable one with larger grain size and hence lower strength, according to the Hall–Petch law [14–16]. Enhancement of the ductility and thermal stability of bulk NC metals is of great importance in materials science.

Alloying UFG and NC metals is one means to increase their ductility and thermal stability while keeping or even further increasing strength [16,17]. Chemical non-homogeneity or/and GB segregations of solute atoms can have a desired effect on the properties of NC metals. GB segregations, depending on various factors, can have a negative effect (e.g., decrease of ductility [18–21] and increase of corrosion [22]) or positive effect (strength enhancement [23]). The negative effects of the GB segregation can manifest themselves even in coarse-grained materials because cracks or corrosion spots can be initiated at a weak GB and easily propagate further. The positive effects can be expected only for metals and alloys having very small grain size and thus a dense GB network. Nowadays, NC metallic materials can be obtained by a number of well-developed techniques [1–4] and the search for the positive effects of GB segregations is timely and promising.

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Due to high vacancy concentration and non-equilibrium GBs having an increased excess energy, alloys subjected to severe plastic deformation (SPD) can have segregations of solute atoms and their clusters in GBs. For instance, Sha et al. [24] observed using three-dimensional atom probe tomography that Mg and Cu atoms in an Al alloy after equal channel angular pressing (ECAP) segregate strongly to its GBs. The formation of GB segregations in Al alloys was observed also after high-pressure torsion (HPT) [25–27]. It has been demonstrated that GB segregations may lead to an additional strengthening of Al alloys [27,28]. For example, Valiev et al. [27] explained the anomalously high value of the strength for UFG Al alloys 7475 and 1570, which positively deviates from the Hall–Petch dependence, by the formation of the GB segregations which suppress dislocation nucleation at GBs due to a solute drag [25].

The solubility level can be greatly increased in non-equilibrium alloys [29]. In a coarse-grained Al alloy, SPD can redistribute alloying elements, lead to their GB segregations [23,30] and result in dissolution of second-phase precipitations or fragmentation of intermetallic compounds [31,32]. The present work, however, does not dwell into discussion how the concentrations and distributions of the alloying elements considered here can be achieved experimentally.

The Hall–Petch law that describes the grain size strengthening of polycrystalline metals and alloys takes into account the behavior of the dislocation ensemble but overlooks the possible change of the deformation mechanisms and GB structure with decreasing grain size. Thus, at average grain size of materials below ~100 nm, the plastic deformation may occur due to the GB sliding (GBS) mechanism which reduces the grain size strengthening. As a result of this process, mechanical properties of the NC materials cannot be described only by the Hall–Petch law [33]. Despite the plastic flow, it is believed that in NC materials, a positive deviation from the Hall–Petch relationship can be observed [27,34]. The additional strengthening effect can be associated with the feature of the GB structure and the dislocation, precipitation or solid solution hardening mechanisms [35–37]. However, NC materials, in particular, NC aluminum alloys, have a low work hardening rate and therefore small contribution of the dislocation hardening mechanism [38].

GB shear (or sliding, GBS) and normal GB motion (or migration, GBM) are often coupled, i.e., they operate simultaneously [39–41]. Simultaneous GBS and GBM are often called shear-coupled migration of GBs [39–42]. These two well-established modes of GB motion can be accompanied by the cooperative GB sliding and shear-coupled migration process which reduces the energy required for the deformation and increases plasticity of polycrystalline materials [43,44]. The shear-coupled migration of GBs can be responsible for the dislocation emission in NC materials [45].

Plastic deformation mechanisms involving GBs have been studied both experimentally and theoretically. It has been supported by the high-resolution transmission electron microscopy (TEM) observation carried out on an Al bi-crystal with a $\Sigma 41$ {5 4 0} GB that GBM occurred due to disconnections resulting from decomposition of lattice dislocations interacting with GBs [46]. The coupling effect between GBS and GBM was observed for various bi-crystals [47–50]. It has been shown that GB structure can strongly influence the value and even change the sign of the coupling factor as well as to affect the shear strength [51]. The scanning electron microscope (SEM) study of the behavior of a tilt–twist GB in Al bi-crystals has revealed shear-stress-driven GBM accompanied by GBS and relative grain rotation [52]. However, under stress, the migration of high-angle low ΣGBs can differ from that of random boundaries, and their stress-driven migration is not necessarily coupled to shear [53]. Mompiou and Legros studied grain growth and rotation in sub-micron grained Al thin films by *in-situ* monitoring of orientation of grains during tensile test combined with TEM [54]. It has been revealed that kinematics of the shear coupled GBM for the coincidence site lattice (CSL) GB can be well explained by the GB displacement shift complete lattice (which is the reciprocal lattice of the CSL) dislocation mechanism [55–58].

Molecular dynamics (MD) simulation was utilized to determine the low-angle GB mobility of [1 1 2] tilt GBs in pure Al [59]. The simulation was also performed to study a $\Sigma 5$ GB in Au bi-crystals subject to a shear deformation parallel to the boundary plane, and it was found that GB migrates perpendicular to the boundary plane coupled to GBS for temperatures below 700 K, while above 1000 K, only GBS occurs [60]. The behavior of GBs in fcc Ni under constant tensile load was studied in the framework of MD with the use of the Cleri–Rosato many-body interatomic potential to demonstrate that GB motion occurs through uncorrelated shuffling of individual atoms or in some cases correlated shuffling of several atoms [61]. Analysis of atomic motion in GBs has been recently performed for NC Al via MD by Hou et al. [62]. In another work, the effect of free surface on coupled GBM and GBS has been addressed in the MD study of NC Al thin films [63]. The importance of GBs in plastic deformation has been stressed in theoretical studies of deformation of NC Al at homologous temperatures of 0.8–0.97 [64] and shock loading of Cu [65].

Few studies have been done on the effect of GB segregations on GBS and GBM. The competition between GBS and GBM in NC Cu with and without GB segregations was studied via by Schafer and Albe with MD simulation [66]. They have found that GB segregations of Nb effectively pinned GBs, thus suppressing GBM and allowing only for GBS. Later, they addressed in more detail the contribution to plasticity from GBS and GBM for NC Cu with segregated Nb or Fe atoms [67]. It was concluded that segregating solutes and their distribution in the GBs not only alter the balance between GBM and GBS, but their precise distribution also governs the contribution of intergranular defects. The phase field method for GB solute segregation in polycrystalline binary alloys was developed by Abdeljawad and Foiles, aiming to provide a quantitative description of the thermodynamic aspects of GB segregations [68].

The existing studies are not clear enough about the deformation mechanisms and mechanical behavior of NC alloys having GB segregations. The present work studies the deformation behavior of NC pure Al and NC binary Al alloys with GB segregations of Co or Mg using MD simulation. The deformation mechanisms of Al in the presence or absence of GB segregations are also studied for bi-crystals with high-angle tilt GBs. As fracture mechanisms are not concerned in this work, to avoid crack nucleation the shear deformation of the materials is modeled in the presence of sufficiently high hydrostatic pressure.

2. Modeling

The matrix element (Al) has the face-centered cubic (fcc) lattice and an atomic radius of 143 pm, while the alloying elements Co and Mg have atomic radii of 125 and 160 pm, respectively [69]. The simulation is conducted using the large-scale atomic/molecular massively parallel simulator (LAMMPS) program package [70]. The interatomic forces are described by the many-body embedded-atom method (EAM) potential [71].

The EAM potential can properly reproduce elastic properties as well as the difference between the vacancy formation and cohesive energy, which cannot be handled by a pair potential [72]. Particularly, the EAM potential for pure Al used in the work provides a good description of the properties of solid Al and its melting properties [73]. For the Al–Mg system, the Finnis–Sinclair potential [74] correctly reproduces both zero-temperature solid properties and solidus and liquidus lines on the Al-rich part of the Al–Mg phase