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Solute effects on interfacial dislocation emission in nanomaterials: Nucleation site competition and neutralization

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ABSTRACT

Solutes added to stabilize nano-crystalline metals against grain growth, may segregate to grain boundaries and triple junctions where they can affect the process of the dislocation emission. We demonstrate that this effect can be very complex due to different rates of segregation at different interfaces. Moreover, at large concentrations, when the solutes form clusters, the interfaces between these clusters and the matrix can introduce new dislocation emission sources, which can be activated under lower applied stress. Thus, the strength maximum can occur at a certain solute concentration: adding solutes beyond this optimal concentration can reduce the strength of the material.

Grain boundaries (GB) serve as obstacles to dislocation motion in conventional materials [1] and as their density increases yield strength increases along with decreasing grain size, according to the classical Hall-Petch relationship. A maximum strength is achieved for very small grain sizes, however, and further reductions in grain size can result in softening due to the activation of interfacially-mediated plasticity mechanisms such as grain boundary sliding and grain rotation [2,3]. Nano-crystalline materials, also suffer from a strong tendency for grain growth and coarsening even at relatively low temperatures, as a result of the extreme driving forces provided by the interfacial energy. These tendencies can be decreased by small solute additions [4,5], which tend to segregate at the grain boundaries, reducing their mobility and suppressing grain boundary mediated plasticity mechanisms [6–11]. However, solutes may also affect the process of dislocation emission from GBs [12] and triple junctions (TJ), which is one of the key mechanisms of plastic deformation at nanoscale grain sizes [13–15]. As grain size, stress and temperature vary, several mechanisms of plastic deformation can be active simultaneously, competitively and/or cooperatively, making it difficult to isolate and study any individual deformation mechanism [7,10,16,17]. Moreover, possible strengthening of nanocrystalline alloys associated with the grain boundary relaxation (e.g., see [18]) makes the picture even more complex. This explains why the effect of solute atoms on dislocation nucleation from GBs has not been systematically studied. We have recently used atomistic simulations to provide direct evidence of the strong effect of solutes segregated at a GB on dislocation nucleation and yield stress under tensile loading [19], using a simple bi-crystal geometry, for which the nucleation and propagation of dislocations from a GB is the only possible mechanism of plastic deformation. While the bi-crystal geometry provides a very convenient way to study the dislocation nucleation from a particular GB, some potentially important aspects of the deformation behavior of real materials are not present when such a geometry is employed [20]. In particular, in a nano-crystalline material under applied stress, dislocation slip can be initiated from multiple competing sources located at GBs and TJs. Therefore, the dependence of the yield stress on the solute concentration can be more complex than revealed by the results we obtained using the bi-crystal geometry in [19].

In the present study we have employed a more complex, yet still tractable multi-grain geometry, previously used in our study of the dislocation nucleation in pure nano-twinned materials [21]. The simulation cell contains different grain and twin boundaries and their triple junctions (see Fig. S1 in [22]). This geometry resembles the microstructure of sputtered thin films produced and tested experimentally [23,24]. The simulation cell contains one type of asymmetric tilt grain boundaries (ATGB), two distinct types of symmetric tilt grain boundaries (STGB), coherent twin boundaries (CTB) and four distinct types of TJs between the GBs and CTBs. Dislocation emission from grain boundaries and triple junctions is the only mechanism of plastic deformation in this system for tensile loads applied in the direction normal to the grain boundaries. Thus the chosen geometry allows to study how different dislocation nucleation sources compete with each other. In the present work, we studied Ag with varying Cu additions. The atomic interactions

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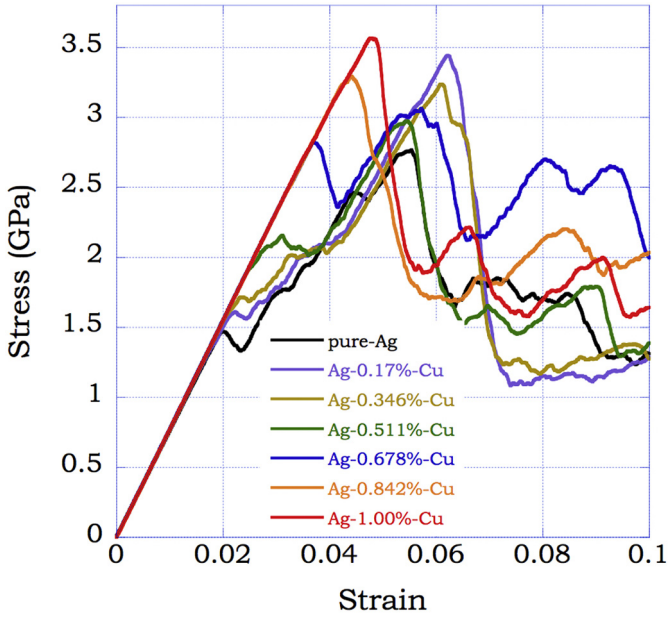

Fig. 1. Stress-strain curves obtained using different solute concentrations (at.%).

were described by an embedded-atom method (EAM) potential developed in [25]. In particular, this potential was fit to the stacking fault energy in pure Ag and provides a reasonable solubility energy for Cu solutes in Ag. Due to the low solubility of Cu in Ag [26], the solutes have a strong tendency for segregation at the GBs and TJs.

All simulations were carried out using the LAMMPS simulation package [27] and the visualization of the simulation snapshots was performed using the software package OVITO [28]. The preparation of the pure Ag model was described in details in [21] and the way to introduce the Cu solute atoms and equilibrate the simulation cell using a hybrid Monte Carlo/molecular dynamics (MC/MD) [29] simulations was described in [19].

Prior to tensile loading, all simulation cells were equilibrated at T = 300 K and zero applied stress. The tensile loading simulations were carried out with a constant engineering strain rate of 10^8 s^{-1}. The deformation was applied in the x-direction (normal to the average GB plane), while the stresses in the other two directions were kept zero. Stress-strain curves obtained for different solute concentrations are shown in Fig. 1. In all cases, the stress first increases with increased applied strain until the emission of the first dislocation. Since the dislocation emission is the only possible mechanism of the plastic deformation in the chosen simulation geometry, the value of the stress at that moment was considered as the yield stress in the present study. The dislocations are emitted

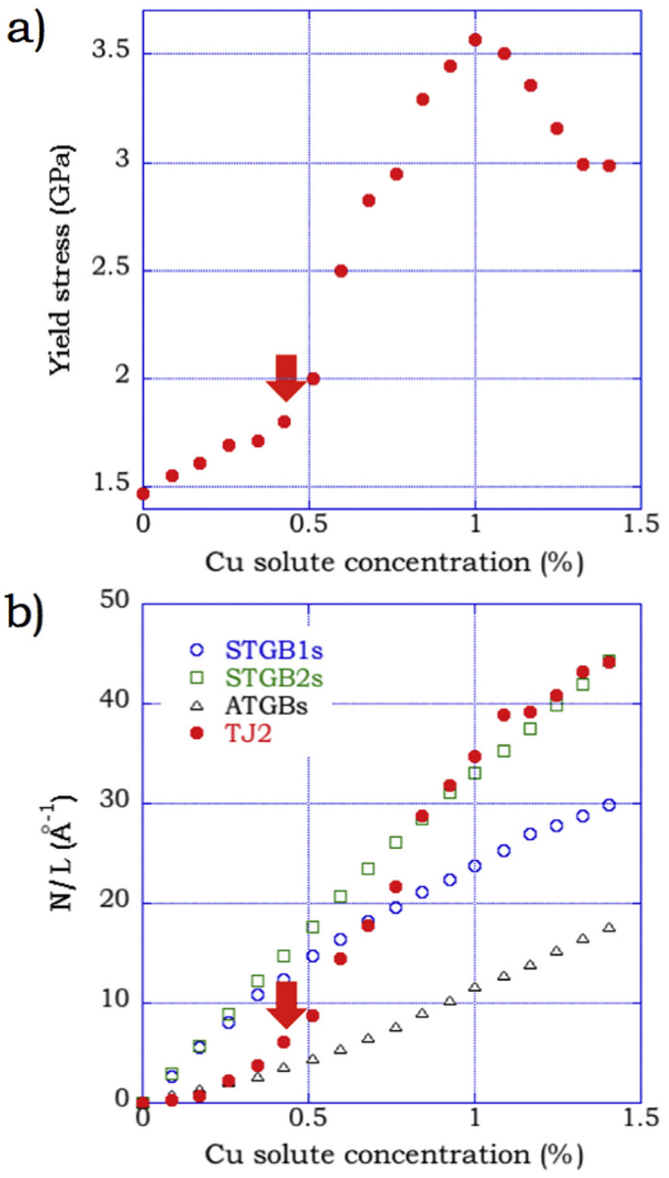

Fig. 3. a) The dependence of the yield stress on solute concentration (at.%). b) The number of solutes per unit of length at different GBs and a TJ. The red arrows indicate the solute concentration at which the yield stress begins to increase rapidly. This is associated with the accelerated segregation of the solutes at the triple junctions, and the corresponding neutralization of the last active dislocation sources located there. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

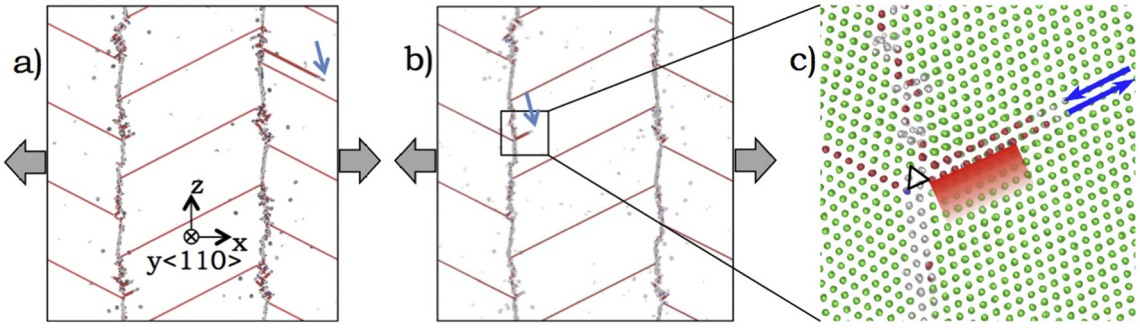

Fig. 2. Examples of dislocation emission from competing sources. The large grey arrows indicate the direction of the applied deformation. The atoms are colored according to the Common Neighbor Analysis (CNA) [32,33]. The color-coding is as follows: green – FCC, red – HCP, grey – other. The small blue arrows highlight the dislocations emitted from a) STGB, and b) TJ (fcc (bulk) atoms are not shown). c) The enlargement of the rectangular segment (all atoms are shown) from b). The triangular structural unit, which serves as a dislocation emission source, is highlighted. The arrows schematically indicate the direction of motion for two atomic planes in the course of dislocation emission. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)