DETERMINING THE RATE-CONTROLLING, GRAIN-BOUNDARY-MEDIATED MECHANISMS IN ULTRAFINE GRAINED AU AND AL FILMS

Sandra Stangebye[1], Lina Daza-Llanos[1], Kunqing Ding[1], Xing Liu[1], Yin Zhang[2], Ting Zhu[1], Josh Kacher[1], Olivier Pierron[1*]

[1]Georgia Tech, Atlanta, GA, USA, [2]MIT, Boston, MA, USA

[*] *Presenting Author email: olivier.pierron@me.gatech.edu*

Abstract

The active grain boundary (GB) mediated mechanisms in ultrafine grained (ufg) Au and Al metallic films, and the extent to which they dictate plastic flow kinetics, are investigated in this work. The approach consists of a synergistic integration of *in situ* transmission electron microscopy (TEM) deformation experiments, nanomechanical testing, and transition state theory based atomistic modeling, in order to provide a linkage between GB-mediated dislocation processes and their deformation kinetics. The *in situ* TEM nanomechanical testing experiments are employed to simultaneously identify plastic deformation mechanisms, obtain key details, and measure the sample-level true activation volume in ufg thin films. The activation of relevant GB mediated dislocation mechanisms is modeled using the atomistic free-end nudged elastic band (FENEB) method as a function of representative, experimentally observed GB characters and local stress. Proper integration of experiments (sample-level true activation volume) and atomistic simulations (activation volumes of dislocation processes) to determine strength/rate-controlling mechanisms requires linking the applied stress to the local stress. To that end, a model of grain-size-dependent activation volume previously developed by Conrad is extended to account for the competition between various GB mediated mechanisms.

Results

Figure 1A shows the microstructure of our 100 nm thick Au films, having an average grain size of 150 nm and a <111> out-of-plane texture. These specimens were tested in the TEM to measure the sample-level activation volume (V^*_{exp}) as a function of applied stress, with and without e-beam (we used our quantitative *in situ* TEM technique to quantify the e beam effects on the measured mechanical properties, and found that the effects were negligible for Au), whose results are summarized in Figure 1B. The average experimental value is 10 b^3 for our Au thin films. The *in situ* TEM observations include isolated dislocation nucleation from GBs and interaction of both perfect and partial dislocations. Figure 1C shows an example of a dislocation cross-slip event leading to a transition between intra- and intergranular glide.

Our FENEB calculations with Au have so far been focused on the nucleation of both surface dislocation and GB dislocation. Overall, a key finding from these FENEB results is that both surface and GB dislocation nucleation are associated with activation volumes larger than $20b^3$ for Au (corresponding to an activation energy of 0.7 eV). To compare our atomistically determined activation volumes with our experimentally measured values from polycrystalline specimens, it is necessary to account for the amplification of local stress at a GB (where the rate-controlling dislocation process is activated) relative to the applied stress on a polycrystal. To this end, we invoke the Conrad model giving a Hall-Petch-like relation of grain size dependent activation volumes. This model evaluates the amplified local stress at the GB by considering the pileup of a dislocation array against this GB. The model is used to show that dislocation nucleation from GB is unlikely the rate-dominant mechanism. Alternative mechanisms based on TEM observations are discussed and their activation volumes are investigated atomistically.

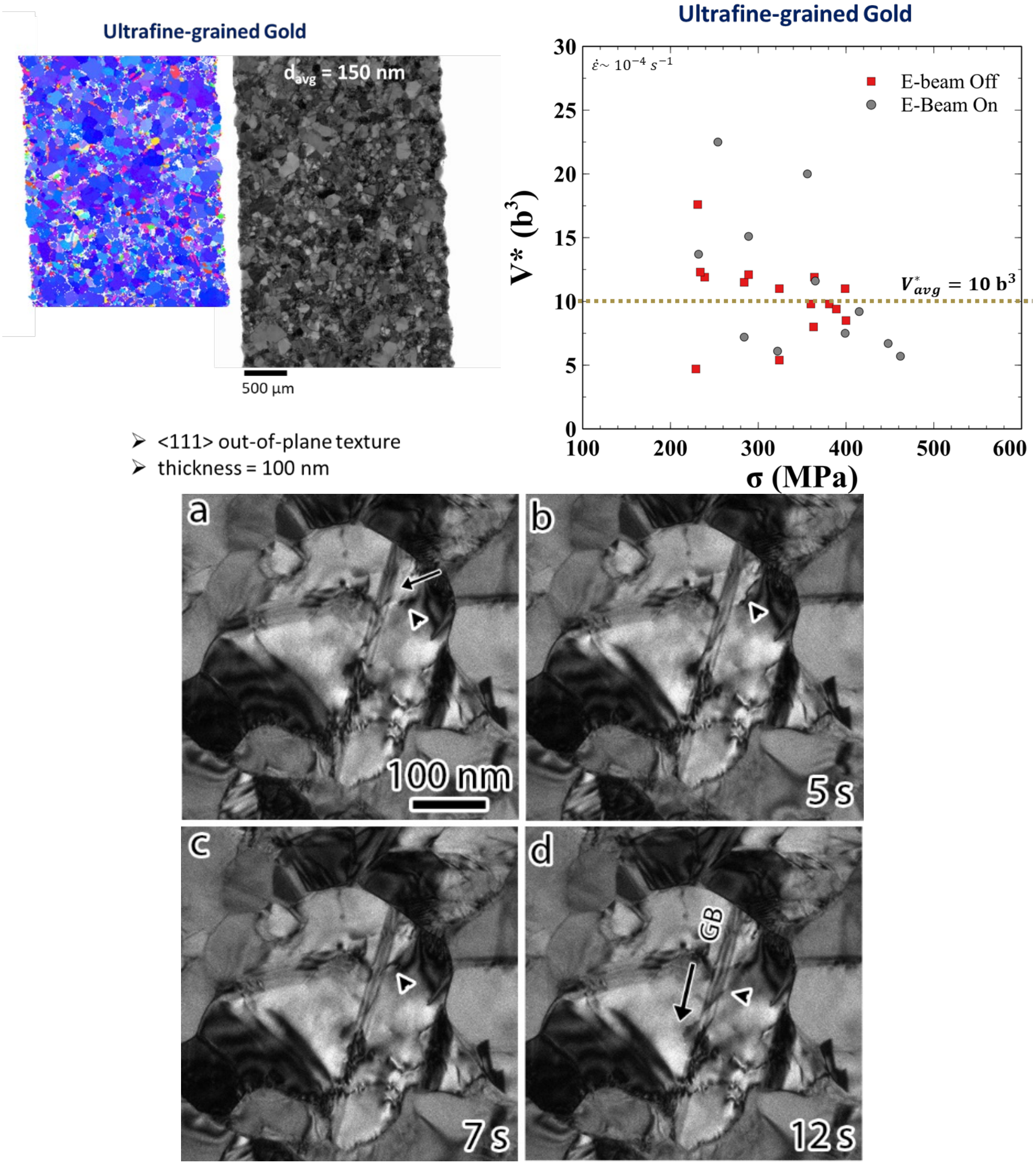

Fig. 1. In situ TEM deformation results. A (Top left) Microstructures of our Au thin films for which V^*_{exp} were measured using in situ TEM experiments. B (Top right) V^*_{exp} as a function of applied stress for Au. C (Bottom left) Frames from in situ TEM video showing dislocation cross-slip and subsequent intergranular glide along boundary plane during stress relaxation. Arrows in (a) and (b) indicate direction of dislocation glide and the arrowhead in each frame track a single dislocation as it cross slips and glides in the boundary. Experiment time is given in each frame.

Acknowledgements

This work is supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES) Materials Science and Engineering (MSE) Division under Award #DE-SC0018960.