Uncovering deformation mechanisms of nanostructured materials

NSF NIRT Grant DMR-0210215
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The reliability of next-generation MEMS, NEMS, magnetic and ultra-hard films, and micro/nano devices, in general, will be closely tied to their mechanical performance. There is and will continue to be a clear need for a fundamental description of the mechanical behavior of these nanocrystalline structures. To be truly predictive, this description must be based on a sound understanding of operative deformation mechanisms, however, the fact that mechanisms have not been clearly identified for nanocrystalline materials is currently exacerbated by the fact that many of the plasticity models that were developed to describe conventional materials are known to break down at these reduced length scales.

The overriding intellectual goal of the current study is to develop a science-based protocol for measuring, describing and modeling deformation and fracture processes in nanocrystalline materials [1]. The interdisciplinary team includes expertise in the synthesis of nanostructured materials, experimental characterization of mechanical properties at small scales, transmission electron microscopy (TEM), and multi-scale modeling. In addition, the Hopkins group has initiated international collaborations with colleagues at Ecole des Mines de Paris (Forest and Saintier) and CEMES/CNRS de Toulouse (Legros) in France.

In this project, the mechanical response of nano-scaled materials is being probed with novel designs for MEMS-based tensile and transient microsample experiments and *in situ* and post mortem TEM observations of high purity nanostructured thin films. Multi-scale finite element calculations, containing physical models that are based on the experimental findings and incorporating adaptive meshing and cohesive elements with atomistic descriptions of grain boundaries in nanocrystalline materials, are being used to study and model the collective macroscopic response of a compilation of nanocrystalline grains. In this way, multi-scale models that are based on experimentally characterized atomic level processes will be used to describe the mechanical behavior of nanocrystalline materials, as measured in micro-scale tensile experiments.

Mechanical response of nanocrystalline materials. In the first year of the project, we have employed microsample tensile testing to measure the mechanical response of nanocrystalline Cu that was prepared by "one-step" processing and shown that nanocrystalline materials can reach impressively high strengths in the absence of porosity [2]. We have also developed the process flow required to make MEMS-based tensile specimens of nanocrystalline Al thin (~250nm) films and conducted preliminary transient experiments. In the latter, stress relaxation tests and strain rate jump tests have been conducted to derive the apparent activation volume and

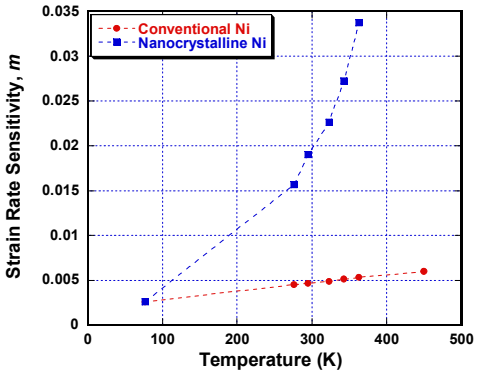

Fig. 1: rate sensitivity of nc- and gc-Ni.

strain rate sensitivity for nanocrystalline Ni produced commercially at Intergran via electrodeposition. This material has an average grain size of about 30nm, thus enabling us to study a fully dense and well-characterized nanocrystalline metal. The magnitude observed for these characteristic parameters, as well as their dependences on deformation temperature, were found to be very different from those of coarse-grained Ni, and the results are being used to support or refute the various rate-limiting deformation mechanisms previously proposed, or suggested by computer simulations, for nanocrystalline metals. For example, the strain rate sensitivity of the flow stress for the nanocrystalline Ni was measured using stress relaxation experiments. The measured values are plotted as a function of temperature and compared with typical values for coarse-grain (cg) Ni in Fig. 1. The dramatic difference in the mechanical response of Ni at these two different grain sizes is one subject of our on-going investigation.

Experimental observations of partial dislocation activity in nanocrystalline Al. To date, our most important finding has involved post mortem TEM observations that provide clear evidence of deformation twinning in plastically deformed nanocrystalline aluminum [3]. The presence of these twins, which are not observed in coarse-grained aluminum, is directly related to the nanocrystalline structure. We have derived a dislocation-based model to rationalize our observations of the presence of deformation twins and stacking faults in nanocrystalline alloys. These findings underscore a transition from deformation that is controlled by normal dislocation activity to one controlled by the emission and subsequent propagation of partial dislocations that are formed at one grain boundary and then traverse the nanocrystalline grains, leaving stacking faults and twins in their wake. The transition from ordinary dislocation glide to this new nanoscale deformation mechanism is predicted and observed to occur when grain size reaches tens of nanometers. These findings are in good agreement with molecular dynamics simulations of deformation processes in nanocrystalline materials, which predict that grain boundary sliding and partial dislocation activity are the active deformation mechanisms in metallic materials with grain sizes on the order of 10-20 nanometers [4].

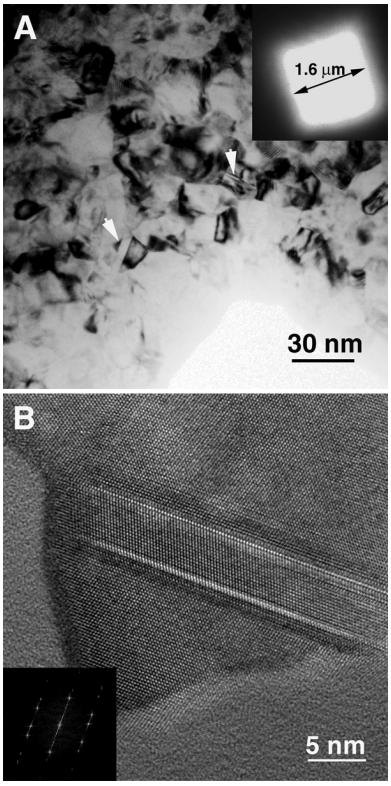

Fig. 2: Experimental TEM observation of twinning in nc-Al.

Multi-scale modeling. Describing the mechanical behavior of a composite of nanocrystalline grains with a model that is based on atomic level deformation processes in a multi-scale problem. Atomistic calculations have been used to analyze the behavior of grain boundaries with applied shear and tensile loads, see Fig. 3 [5]. For shear, these calculations revealed a three-plateau regime, which is independent of grain boundary (GB) type. To date, most work on GB sliding has assumed rigid grain motion without atomic relaxation and resulted in unrealistically high estimates of shear strength (regime I). Simulations in which all atomic planes were allowed to relax and move resulted in the emission of partial dislocations from the boundary (regime III), which is in excellent agreement with our TEM observations [3] and previous atomistic simulations [4] but tells us very little about grain boundary sliding. Restricting the number of

atomic planes that were relaxed shut off partial dislocation emission, resulted in atomic shuffling near the GB, and allowed us to separate GB sliding from intragranular plasticity (regime II). The establishment of the atom shuffling plateau in regime II is currently being used to obtain the cohesive law behavior of a variety of grain boundaries. A non-local crystal plasticity model will be developed later and tested in this project. In this novel model, the sources of dislocations will be related to free volume creation at grain boundaries, which in turn may be associated, for each GB type, to an average GB slip.

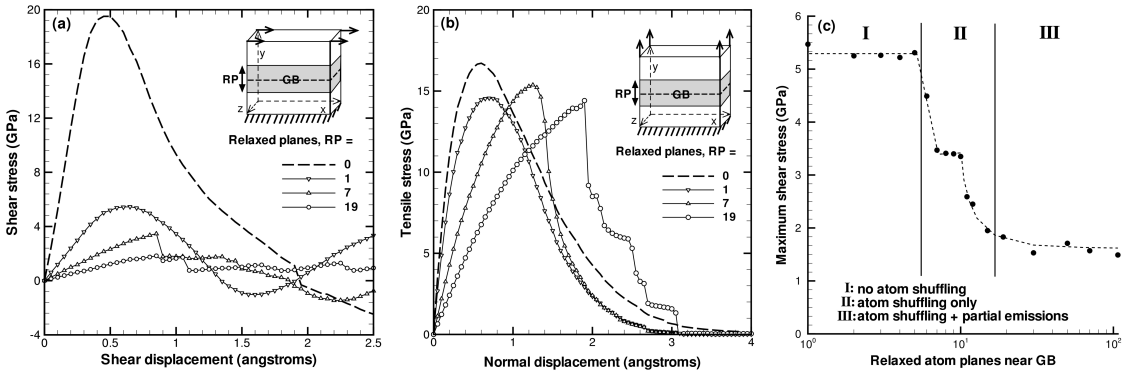

Fig. 3: Influence of {221} GB plane relaxation on local constitutive relations for a Cu Σ9(221) boundary in (a) shear and (b) tension. (c) Maximum shear stress versus number of relaxed GB planes and the three regimes.

At the continuum level, a Voronoi tessellation technique has been developed to automatically mesh microstructures with grain size distributions in close agreement with experimental measurements. The GB cohesive laws are integrated into the mesh within a contact algorithm, and particular attention has been devoted to resolving the challenging multibody-dynamics numerical problem that takes place at triple junctions. This was achieved by modifying traditional master slave algorithms, e.g. by considering a weighted average over a time step of the predictions with all grains being alternatively as master and slave. Simulations of GB sliding in nanocrystalline Cu evidence very heterogeneous sliding and stress distributions, but averaging over a reasonable compilation of grains has allowed us to generate a corresponding macroscopic quasi-plastic behavior that can be compared with the microsample tensile experiments. These advancements in both our understanding of GB sliding as well as algorithmic developments open the door to parametric studies. One may for instance use the methodology to investigate what are the grain size distributions that maximize ductility while preserving high strength.

References

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[2] Y.M. Wang, K. Wang, D. Pan, K. Lu, K.J. Hemker E. Ma, "Microsample tensile testing of nanocrystalline copper", *Scripta materialia* **48** (2003) 1581-1586.

[3] Mingwei Chen, En Ma, Kevin J. Hemker, Hongwei Sheng, Yinmin Wang, Xuemei Cheng, "Deformation Twinning in Nanocrystalline Aluminum", *Science*, **300** (2003) 1275-1277

[4] H. Van Swygenhoven, P.M. Derlet, A. Hasnaoui, *Phys. Rev. B*, **66** (2002) 024101.

[5] F. Sansoz, J.F. Molinari, "Incidence of atom shuffling on the shear and decohesion behavior of a symmetric tilt grain boundary in copper", *Scripta materialia*, submitted.