Mechanics of Nanoporous Metals

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Scientific Thrust Area: Nanoscale Electronics and Mechanics

Proposal Titles: Determining the mechanisms of plastic deformation of metallic nanofoams by atomistic simulations (Michael J. Demkowicz, MIT); Thermal phenomena in micro- and nano systems (Leslie Phinney and Patrick E. Hopkins, SNL).

Research Achievement:

We have synthesized a variety of nanoporous metal films, such as pure Au, pure Pt, and Pt-Ni alloys, by electrochemical dealloying of amorphous metal-silicide films that were either magnetron sputtered or electron beam co-evaporated on a silicon substrate. Electrochemical dealloying selectively etches Si and the remaining metal(s) reorganize to form a three-dimensional porous network where both the ligaments and open cell pores are nanometer-scale. For example, for 20 at.% Pt-80 at.% Si films, the average pore and ligament sizes were 20 nm and 15 nm respectively. The Pt ligaments in these nanoporous films were polycrystalline with a grain size on the order of 5 – 10 nm. Our study has focused on understanding the correlation between synthesis parameters and nanoporous morphologies, mechanical properties, and irradiation stability. The two user projects on nanoporous metals are focused on atomistic modeling of deformation behavior and measurement of thermal properties, respectively.

The key achievements are summarized below:

- Three distinct morphologies (one isotropic and two anisotropic) are reported that depend on the composition and surface topology of the alloy prior to dealloying. There are two levels of anisotropy: micron sized features in the range of 0.1 μm to ~1 μm forming a hyperstructure of either convex or concave features on the free surface. Within each hyperstructure, a 3-D network of polycrystalline Pt ligaments (5-30 nm in length, 5nm grain size) and pores (5-30 nm in size) form. A processing-structure map is developed to correlate np-Pt morphology to the processing conditions, showing that the morphology of the np metal can be controlled by patterning the surface of the as-synthesized alloy prior to dealloying.

- The mechanical properties of nanoporous metal films are investigated through nanoindentation, including compression testing of focused-ion-beam machined micro-pillars, and compared to the properties of fully dense metals as well as macro-scale metallic foams. The dependence of strength is studied as a function of film density as well as ligament size to gain insight on the length scale effects. We observe ultra-high strengths in nanoporous metal films that are not explained by the scaling laws for the strength of bulk metallic foams as a function of foam density (Fig. 1).

- Atomistic modeling is being used by a CINT user to study the unusual nanomechanical behavior of nanoporous metals observed in our experiments. Fig. 2 shows a one million-atom

simulation of a np-Au structure with 3 nm ligament diameter. MD simulation results show that the volume-adjusted yield stress of np-metals is nearly two orders of magnitude higher than that of bulk, single crystal metals. Furthermore, MD simulation show that the onset of plastic yielding in np-metals involves nucleation of plasticity events from free surfaces, as opposed to propagation of pre-existing defects in bulk.

- Ion irradiation (Ne ions, 1 dpa) experiments show insignificant radiation damage in np-metals whereas single crystal full-density films show bubbles and defect agglomerates. Presumably the radiation-induced defects migrate to the surface sinks in np-metals.

Future Work

- Study of ion transport through supported lipid membranes on nanoporous metal films (collaboration with Andrew Dattelbaum, Nano/bio thrust).
- Thermal transport measurements in np-metals using a pump-probe transient thermo-reflectance technique (user project).
- Use of Cantilever Array Discovery Platform^{TM} at CINT to measure the energy dissipation mechanisms in np-metals (collaboration with John Sullivan).
- *In situ* straining in TEM to understand the surface-mediated plasticity in np-metals (collaboration with Jianyu Huang).

Publications

1. J.C. Thorp, K. Sieradzki, L. Tang, P.A. Crozier, A. Misra, M. Nastasi, D. Mitlin, S.T. Picraux, Applied Physics Letters, 88, p.33110-116 (2006).
2. A. Antoniou, D. Bhattacharyya, J.K. Baldwin, P. Goodwin, M. Nastasi, S.T. Picraux, A. Misra, Applied Physics Letters, in review.

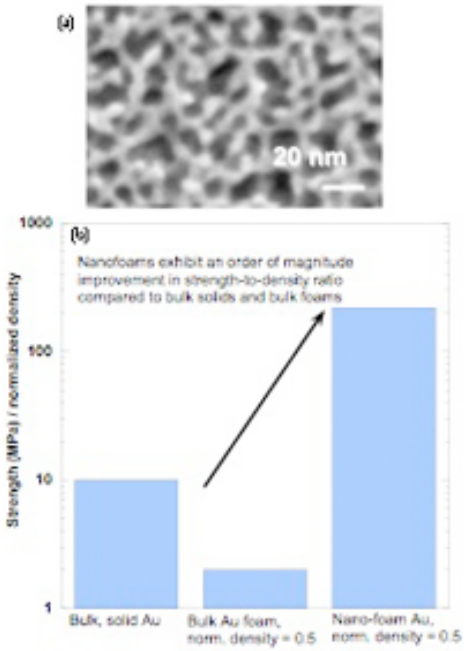

Figure 1 (a) SEM micrograph of a Pt nano-foam; (b) Histogram showing the significant increasing in strength of a nano-foam compared to bulk foam and solid bulk metal.

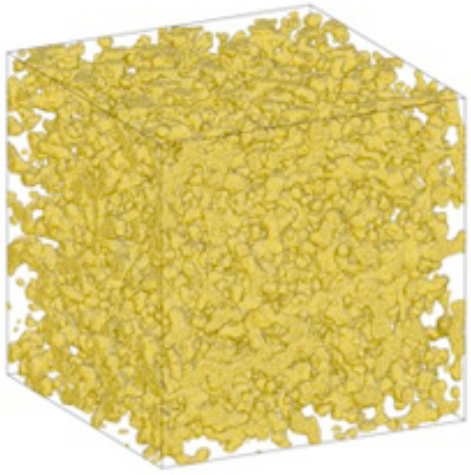

Fig. 2 Computer generated 3-D structure of np-Au. The simulated structure contains 1 million atoms and has 3 nm diameter ligaments.