

Deformation Mechanisms in Nanocrystalline/Ultra-fine grained Materials

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Abstract

Developments in technologies in the leading industrial areas such as aircraft structures, gas turbine technology and automobile industry is highly limited by the materials. The enhanced materials to withstand extreme environment is the key to the advancements. Mainly engineering materials in particular aluminum and magnesium alloys with particle strengthened are essential to withstand high temperature applications. Moreover the discovery of novel materials such as ufg/nanocrystalline exhibiting anomalous behavior lead to huge gap in our understandings of materials. Observations of Glieter et al. [1] that nanocrystalline material exhibits enhanced mechanical responses has lead to various scientific advancements in the material behavior over the past few decades. In the recent past the focus in the research community shifted to the mechanics of the material deformation rather than the phenomenological models. Investigations at the grain-level from atomistic simulations and high quality microscopic elucidates our understandings of governing deformation mechanisms. But one has to correlate all the underlying micro-mechanisms to the properties of the macroscopic properties of the materials. In this attempt we at Brown develop multi-scale simulations and scale bridging models. In particular in our lab we perform continuum and meso-scale simulation and rely on other groups for atomistic calculations to tailor the materials for enhanced properties.

In my due course of grad studies under the guidance of Prof. Allan Bower, I had the opportunity to work on the couple of projects on which my talk will be focused as listed. (a) Intergranular strain evolution in nanocrystalline materials. This study is an attempt to quantify the contributions from different mechanisms in a manner which can be readily experimentally verified using neutron/X-ray diffraction techniques. We use crystal-plasticity and interface diffusion modeling techniques to simulate the dislocation creep and diffusional

creep behavior in the solid. We systematically showed that the well known behavior of nanocrystalline materials exhibiting both Hall-Petch and Inverse Hall-Petch effect. To probe the underlying grain-level(microscopic) deformations we computed the intergranular strain. We found a good match with the available experimental observations. We also observed that intergranular strain which is a measure of plastic anisotropy shows a neat trends in different deformation dominated regimes and a clear transition between deformations mechanisms. In particular intergranular strain vanishes in the grain boundary sliding regime [2]. (b) Discrete dislocations simulations in ufg materials. These are meso-scale simulations which unlike atomistic simulation has relaxed temporal and spatial limitations. This feature realistically(to certain extent) enables to tailor made materials. These simulation has control over micro-structural properties such as grain size, grain boundary chemistry, structure and energy etc. Which enables to simulate novel materials with unparalleled performance. Even though DD simulations has relaxed spatial and temporal restrictions as compared to atomistic simulations the current computing power is highly limiting its applicability. To address this issue we adopted the fast multi-pole multi-pole method to compute dislocation-dislocation interactions. Using this method we drastically reduced the computing time without loss of accuracy and precision. Further work is being carried out in an attempt to tailor made composites.

References

- [1] R. Birringer, U. Herr and H. Gleiter, Suppl. Trans. Japan Inst. Metals 27, 43 (1986).
- [2] V. Chinthapenta, Y. Gao, Y. Wei and A. F. Bower, Numerical simulations of intergranular strain evolution in nanocrystalline materials, Unpublished 2011.