8th. World Congress on Computational Mechanics (WCCM8)
5th. European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2008)
June 30 – July 5, 2008
Venice, Italy

PLASTICITY IN NANOCRYSTALLINE METALS: A MOLECULAR DYNAMICS STUDY

***P. M. Derlet[1] and H. Van Swygenhoven[3]**

[1]Materials Science and Simulation, ASQ/NUM, Paul Scherrer Institut, Switzerland
peter.derlet@psi.ch
mss.web.psi.ch

[2] Materials Science and Simulation, ASQ/NUM, Paul Scherrer Institut, Switzerland
helena.vanswygenhoven@psi.ch
mss.web.psi.ch

Key Words: *atomistic simulations, bulk metallic nanocrystals, plastic deformation.*

ABSTRACT

The use of large scale molecular dynamics to study the mechanical properties of FCC nc metals provides a detailed picture of the atomic-scale processes during plastic deformation at room temperature. Simulations have revealed interface dominated processes such as grain boundary sliding and migration, and intragranular deformation processes involving dislocation activity [1]. In the absence of defects within the grain interior it has been found that grain boundaries can act as both sources and sinks for partial or full dislocations and that the surrounding grain boundary environment can significantly affect the motion of a dislocation as it propagates through the grain [2]. An aspect making it difficult to compare with experiment is the short time scale restriction of the molecular dynamic's technique, where the typical strain rates used till now have been of the order of 10^9/sec to 10^8/sec. With continuing increases in computational power it now becomes possible to not only simulate larger atomic configurations, but also for a longer physical times or at reduced the strain rates.. The present work shows that simulating deformation at a constant strain rate of 10^7/sec on nc Al samples with a mean grain size is 10 nm, reveals new aspects of the deformation mechanism. Analysis in terms of slip accumulation within grains and local strain both within the grains and at the grain boundary will be presented and discussed in terms of previous simulation work.

REFERENCES

[1] H. Van Swygenhoven, P. M. Derlet and A. G. Frøseth, "Nanocrystalline metals: stacking fault energies and slip", Nature Mater. 3, 399 (2004).

[2] H. Van Swygenhoven, P. M. Derlet and A. G. Frøseth, "Nucleation and propagation of a dislocations in nanocrystalline fcc metals". Acta Mater. 54, 1975 (2006).