A finite element study of the mechanical behavior of nanocrystalline fcc metals

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Nanocrystalline metals are polycrystalline metallic materials with grain sizes typically less than 100 nm. These materials have been the subject of intense, world-wide research over the past two decades, and due to this research activity the micro-mechanisms governing their macroscopic mechanical behavior are now beginning to be better understood. The following features of the operative micromechanisms are now reasonably widely-accepted [1-4]: (1) There is a strong interplay between dislocation-based deformation in the crystalline grain interiors and the inelastic deformation mechanisms operative in the grain-boundary regions. (2) Grain boundaries acts as both sources and sinks for dislocations. (3)There exists a critical grain size d_c, above which plastic deformation in nanocrystalline grain interiors occurs by the emission of *complete dislocations* from grain boundaries, and below which the plastic deformation occurs by *partial dislocations*. The partial dislocations produce stacking faults as they glide through the grains [5,6].

We have developed a finite-element-based "core-and-mantle" type two-dimensional model to numerically study the deformation and failure behavior of nanocrystalline fcc metals. A rate-dependent amorphous plasticity model [7] which accounts for cavitation and related failure phenomena is used such to model the grain boundary, while a crystal plasticity model which accounts for the transition from partial dislocation to complete dislocation mediated plasticity is used for the limited plasticity of the grain-interiors. Numerical simulations using material parameters estimated to represent the macroscopic rate-dependent stress-strain response of nanocrystalline Nickel (nc-Ni) show that here is a deformation mechanism transition from grain-interior dominant shearing to grain boundary dominant shearing as the average grain-size decreases from 50 nm to 10 nm, and that the low ductility in nc-Ni is the result of intergranular failure due to grain boundary shearing and resulting cavitation at triple-junctions and other high stress points in the microstructure. Our numerical simulations also show that the strength of nc-Ni is expected to be slightly higher in compression than in tension, primarily due to the easier operation of cavitation failure of the grain boundaries in tension.

References

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