Phase Mixture Model and Finite Element Simulation of Nanostructured Metals

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As nanostructured materials (NSMs) are becoming a major focus of materials research, the attention of materials scientists and engineers is turning to their mechanical performance. In contrast with conventional coarse grained materials, which are either strong or ductile but rarely both strong and ductile, it is expected that a combination of high strength and ductility can be achieved with NSMs. In some cases, this was confirmed by experimental studies. In spite of the significant interest and efforts in establishing the mechanical properties of NSMs, deformation mechanisms underlying their plastic deformation (and even elastic deformation) are not well understood yet. In this study, the deformation mechanisms of NSMs of various grain sizes were investigated as a function of temperature and strain rate. The work has been model-driven and has provided a description of the phenomenology and the mechanisms underlying the mechanical properties of NSMs. Common to the proposed models is the concept of a 'phase mixture' in which the grain boundaries are treated as a separate phase. The volume fraction of this 'phase' may be quite appreciable in an NSM. Based on the theoretical model that provides an adequate description of the grain size dependence of elasticity and plasticity covering all grain size ranges - from coarse grain size down to the nanoscale - the tensile deformation response of NSMs was investigated. In the talk summarizing this study, various deformation regimes will be discussed in terms of 3D deformation mechanism maps represented in the strain rate/temperature/grain size space. The model is essentially a multi-scale one, in that processes at atomic diffusion and dislocation glide level are incorporated in a continuum model. The phase mixture model was implemented in a finite element code used for simulation of uniaxial tensile deformation of nanomaterials.

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