Nanograin Promote Dynamic Shear Localization

Adiabatic shear failure is a dynamic ductile failure mechanism that is characterized by the development of a narrow band, known as an Adiabatic Shear Band (ASB). ASB is the result of intense shear localization casing noticeable material softening, followed by catastrophic failure. Interestingly, the observation of dynamically recrystallized nanograin(NG) in ASBs leads in recent to a new hypotheses about the origin of ASBs. The experimental observation that the deformed microstructure of Ti6Al4V comprised NGs prior to ASB formation brings with it the question whether the dynamically formed NGs are at the origin to the ASB formation. In this work, we present a computational study to examine if the presence of NGs in the crystal may give rise to formation of ASBs. While a full microstructural-based model for ASB formation is still far from being accomplished, we limit ourselves to the problem of embedded NGs at predeterminded sites in a loaded single crystal. Such a model allows us to gain insight on how the NGs distribution affects the deformation. To model the system, we performed large-scale molecular dynamics (MD) simulations of Mg lattices with different distributions of NGs. A tensile strain is applied to the computational cell and both the mechanical response and microstructural evolution is tracked during the simulation. In all simulations, we identify four distinct stages in the calculated stress-strain curves: an elastic regime, a region in which the tensile stress remains constant, a hardening stage and finally softening. The microstructural evolution in each stage is identified and is discussed during the talk. In particular, dislocations nucleate at the hardening stage on grain boundaries and glide outside the NG’s into the crystal. Softening commences when these dislocations are absorbed in the neighboring NGs. In result, the strain at which materials softens depends on the density of NGs along active slip planes. If such a path of active slip planes is found, the deformation is localized along this path. Based upon the simulations we propose that the shear localization evolves as percolative process of deformation zones between nanograins. The presence of nanograin is a necessary condition to relieve some of the elastic energy by dislocation emission and absorption. Moreover, the density and spatial arrangement of those grains are of prime importance to accelerate or delay the formation of a strong localization path.