The role of heterogeneous deformation on damage nucleation at grain boundaries in single phase metals

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Abstract: The mechanical response of engineering materials evaluated through continuum fracture mechanics typically assumes that a crack or void initially exists, but it does not provide information about the nucleation of such flaws in an otherwise flawless microstructure. How such flaws originate, particularly at grain (or phase) boundaries is less clear. Experimentally, “good” vs. “bad” grain boundaries are often invoked as the reasons for critical damage nucleation, but without any quantification. The state of knowledge about deformation at or near grain boundaries, including slip transfer and heterogeneous deformation, is reviewed to show that little work has been done to examine how slip interactions can lead to damage nucleation. A fracture initiation parameter developed recently for a low ductility model material with limited slip systems provides a new definition of grain boundary character based upon operating slip and twin systems (rather than an interfacial energy based definition). This provides a way to predict damage nucleation density on a physical and local (rather than a statistical) basis. The parameter assesses the way that highly activated twin systems are aligned with principal stresses and slip system Burgers vectors. A crystal plasticity - finite element method (CP-FEM) based model of an extensively characterized microstructural region has been used to determine if the stress-strain history provides any additional insights about the relationship between shear and damage nucleation. This analysis shows that a combination of a CP-FEM model augmented with the fracture initiation parameter shows promise for becoming a predictive tool for identifying damage-prone boundaries.