ABSTRACT

Physics Based-crystal Plasticity Modeling of Single Crystal Niobium

By

Tias Maiti

Crystal plasticity models based on thermally activated dislocation kinetics has been successful in predicting the deformation behavior of crystalline materials, particularly in face-centered cubic (fcc) metals. In body-centered cubic (bcc) metals success has been limited owing to ill-defined slip planes. The flow stress of a bcc metal is strongly dependent on temperature and orientation due to the non-planar splitting of a/2 (1 1 1) screw dislocations. As a consequence of this, bcc metals show two unique deformation characteristics: (a) thermally-activated glide of screw dislocations - the motion of screw components with their non-planar core structure at the atomistic level occurs even at low stress through the nucleation (assisted by thermal activation) and lateral propagation of dislocation kink pairs; (b) break-down of the Schmid Law, where the dislocation slip is driven only by the resolved shear stress.

Since the split dislocation core has to constrict for a kink pair formation (and propagation), the non-planarity of bcc screw dislocation cores entails an influence of (shear) stress components acting on planes other than the primary glide plane on their mobility. Another consequence of the asymmetric core splitting on the glide plane is a direction-sensitive slip resistance, which is termed twinning/atwinning sense of shear and should be taken into account when developing constitutive models.

Modeling thermally-activated flow including the above-mentioned non-Schmid effects in bcc metals has been the subject of much work, starting in the 1980s and gaining
increased interest in recent times. The majority of these works focus on single crystal deformation of commonly used metals such as Iron (Fe), Molybdenum (Mo), and Tungsten (W), while very few published studies address deformation behavior in Niobium (Nb). Most of the work on Nb revolves around fitting parameters of phenomenological descriptions, which do not capture adequately the macroscopic multi-stage hardening behavior and evolution of crystallographic texture from a physical point of view. Therefore, we aim to develop a physics-based crystal plasticity model that can capture these effects as a function of grain orientations, microstructure parameters, and temperature.

To achieve this goal, first, a new dilatational constitutive model is developed for simulating the deformation of non-linear geometries (foams or geometries with free surfaces) using the spectral method. The model has been used to mimic the void-growth behavior of a biaxially loaded plate with a circular inclusion. The results show that the proposed formulation provides a much better description of void-like behavior compared to the pure elastic behavior of voids. Using the developed dilatational framework, periodic boundary conditions arising from the spectral solver has been relaxed to study the tensile deformation behavior of dogbone-shaped Nb single crystals.

Second, a dislocation density-based constitutive model with storage and recovery laws derived from Discrete Dislocation Dynamics (DDD) is implemented to model multi-stage strain hardening. The influence of pre-deformed dislocation content, dislocation interaction strengths and mean free path on stage II hardening is then simulated and compared with in-situ tensile experiments.