Experimental evidence and first-principles verification of deformation of basal twist grain boundaries in Ti

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Abstract

Titanium (Ti) alloys are high performance materials used in many applications requiring lightweight, strength, and corrosion resistance. Increasing severity of in-service conditions and extended lifetimes are important objectives from the viewpoint of structural applications. Fatigue failure, as a result of repeated mechanical loadings, is a critical design concern for metallic alloys, and Ti alloys in particular. As a result of the improvement of industrial practices, forged components are generally free of defects such as pores or non-metallic inclusions. Instead, microstructural characteristics, including microtexture, and multimodal size distribution of α precipitates, determine the resistance to crack nucleation and the fatigue performance in the high-cycle fatigue regime. Recent experimental results provided evidence of fatigue crack nucleation along basal planes in equiaxed α particles , while cracks lying along prismatic planes were more rarely reported. The associated mechanism was recently revisited to suggest a critical role of Basal Twist Grain Boundaries (BTGBs) located in clusters of equiaxed α grains. These microstructure configurations are composed of two hexagonal close-packed α crystals rotated about the (0001) axis and separated by a grain boundary parallel to (0001) planes. BTGBs are planar α/α grain boundaries where no β phase, or detectable elemental segregation is present. While the competition with other crack nucleation mechanisms is still a subject of discussion, broad relevance was demonstrated considering a variety of alloys and loading conditions. In particular, recent investigations suggested that the high variability in fatigue lifetimes in Ti alloys reported in prior studies could be related to the low density of BTGBs found in engineering microstructures. To clarify the origin of this critical behavior, the mechanical response of bicrystal micropillars containing BTGBs was characterized by means of micropillar compression tests. This approach ruled out any contribution of the microstructural environment, which is difficult to assess in polycrystalline samples. Also, the reference behavior associated with the onset of conventional intragranular slip activity was extracted using single-crystal micropillars for comparison. Afterwards, the deformation mechanisms around the BTGB were analyzed by means of high-resolution scanning and transmission electron microscopy. I. It was found that shear deformation occurred by the glide of one basal grain over the other basal grain at very low values of the critical resolved shear stress (45 - 205 MPa), much lower than that of basal slip (400 - 600 MPa). To

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understand this mechanism, the Grain Boundary Energies (GBEs) of coincident site lattice BTGBs with different twist angles were determined by means of first-principles calculations of supercells. It was found that the GBE variations with respect to twist angle and in-plane translation were negligible for all coincident site lattice BTGBs investigated, leading to a very low shear resistance.