Mechanical Engineering Doctoral Defense

Multiscale Modeling of Oxygen Impurity Effects on Macroscopic Deformation and Fatigue Behavior of Commercially Pure Titanium

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abstract

In this dissertation, first we examine the role of oxygen on various slip planes in α-Ti through generalized stacking fault energies (GSFE) computed using first principles calculations. Then the Peierls-Nabbaro model is utilized in conjunction with the GSFE to estimate the Peierls stress ratios for different slip systems. Using that information, the parameters of the presented continuum crystal plasticity model, namely the critically resolved shear stress (CRSS) values of different slip systems, are calibrated. Further, a set of tension and compression experiments are carried out to obtain the global response of the samples at room temperature in the presence of different concentrations of oxygen and compare them with the crystal plasticity simulations results. The results reveal that compared to the prismatic slip, oxygen enhances CRSS for basal and a-type pyramidal slip systems, while that of the first and second order pyramidal <c+a> slip systems are decreased. Moreover, it is shown that using the presented hierarchical approach, the strengthening due oxygen can be captured with a reasonably good accuracy. The effect of oxygen impurity on titanium is further investigated under high cycle fatigue loading. For that purpose, a two-step hierarchical crystal plasticity for fatigue predictions is presented. Fatigue indicator parameter is used as the main driving force in an energy-based crack nucleation model. To calculate the FIPs, high-resolution full-field crystal plasticity simulations are carried out using spectral solver. A nucleation model is proposed and calibrated by experimental data for two titanium alloys with different oxygen contents. Overall, we show that the presented approach is capable of predicting the high cycle fatigue nucleation time reasonably well.

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