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Finite Element Modeling of Global Ti-6Al-4V Mechanical Behavior in Relationship with Microstructural Parameters

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Abstract : The global mechanical behavior of materials is strongly linked to their microstructure, especially their crystallographic texture and their grains morphology. These material aspects determine the mechanical fields character (heterogeneous or homogeneous), thus, they give to the global behavior a degree of anisotropy according the initial microstructure. For these reasons, the prediction of global behavior of materials in relationship with the microstructure must be performed with a multi-scale approach. Therefore, multi-scale modeling in the context of crystal plasticity is widely used. In this present contribution, a phenomenological elasto-viscoplastic model developed in the crystal plasticity context and finite element method are used to investigate the effects of crystallographic texture and grains sizes on global behavior of a polycrystalline equiaxed Ti-6Al-4V alloy. The constitutive equations of this model are written on local scale for each slip system within each grain while the strain and stress mechanical fields are investigated at the global scale via finite element scale transition. The beta phase of Ti-6Al-4V alloy modeled is negligible; its percent is less than 10%. Three families of slip systems of alpha phase are considered: basal and prismatic families with a burgers vector <a> and pyramidal family with a <c+a> burgers vector. The twinning mechanism of plastic strain is not observed in Ti-6Al-4V, therefore, it is not considered in the present modeling. Nine representative elementary volumes (REV) are generated with Voronoi tessellations. For each individual equiaxed grain, the own crystallographic orientation vis-à-vis the loading is taken into account. The meshing strategy is optimized in a way to eliminate the meshing effects and at the same time to allow calculating the individual grain size. The stress and strain fields are determined in each Gauss point of the mesh element. A post-treatment is used to calculate the local behavior (in each grain) and then by appropriate homogenization, the macroscopic behavior is calculated. The developed model is validated by comparing the numerical simulation results with an experimental data reported in the literature. It is observed that the present model is able to predict the global mechanical behavior of Ti-6Al-4V alloy and investigate the microstructural parameters' effects. According to the simulations performed on the generated volumes (REV), the macroscopic mechanical behavior of Ti-6Al-4V is strongly linked to the active slip systems family (prismatic, basal or pyramidal). The crystallographic texture determines which family of slip systems can be activated; therefore it gives to the plastic strain a heterogeneous character thus an anisotropic macroscopic mechanical behavior. The average grains size influences also the Ti-6Al-4V mechanical proprieties, especially the yield stress; by decreasing of the average grains size, the yield strength increases according to Hall-Petch relationship. The grains sizes' distribution gives to the strain fields considerable heterogeneity. By increasing grain sizes, the scattering in the localization of plastic strain is observed, thus, in certain areas the stress concentrations are stronger than other regions.

Keywords : microstructural parameters, multi-scale modeling, crystal plasticity, Ti-6Al-4V alloy
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