Study of 3-D stress development in parent and twin pairs of a hexagonal close-packed polycrystal: Part II - Crystal plasticity finite element modeling - DTU Orbit (25/12/2018)

Study of 3-D stress development in parent and twin pairs of a hexagonal close-packed polycrystal: Part II - Crystal plasticity finite element modeling

Stress heterogeneity within each individual grain of polycrystalline Zircaloy-2 is studied using a crystal plasticity finite element (CPFE) model. For this purpose, the weighted Voronoi tessellation method is used to construct 3D geometries of more than 2600 grains based on their center-of-mass positions and volumes as measured by three-dimensional X-ray diffraction (3DXRD) microscopy. The constructed microstructure is meshed with different element densities and for different numbers of grains. Then a selected group of twin and parent pairs are studied. It is shown that the measured average stress for each grain from the 3DXRD experiment is within the stress variation zone of the grain modeled in the CPFE simulation. Also, the CPFE average stress calculation for each grain is in good agreement with the measured average stress values. It is shown that upon considering the stress variations within each grain, stresses in the parent and twin are quite different if they are plotted in the global coordinate system. However, if the stress tensor is rotated into the local coordinate system of the twin habit plane, all the stress components averaged over the presented population are close, except for the shear acting on the twin plane and the transverse stress. This result is significant as it provides information needed to model such parent-twin interactions in crystal plasticity codes.

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